Optimized and Quasi-Optimal Schwarz Waveform Relaxation for the One Dimensional Schrödinger Equation

Laurence Halpern, Jérémie Szeftel

Optimized and Quasi-Optimal Schwarz Waveform Relaxation for the One Dimensional Schrödinger equation

Laurence Halpern* Jérémie Szeftel‡

May 6, 2006

AMS subject classifications. 35J10, 58J40, 65M12, 66M55

Abstract

We design and study Schwarz Waveform relaxation algorithms for the linear Schrödinger equation with a potential in one dimension. We show that the overlapping algorithm with Dirichlet exchanges of informations on the boundary is slowly convergent, and we introduce two new classes of algorithms: the optimized Robin algorithm and the quasi-optimal algorithm. We study the well-posedness and convergence, in the overlapping and the non overlapping case, for constant or non constant potentials. We then design a discrete algorithm, based on a finite volumes approach, which permits to obtain convergence results through discrete energies. We also present a quasi-optimal discrete algorithm, based on the transparent discrete boundary condition of Arnold and Ehrhardt [1]. Numerical results illustrate the performances of the methods, even in the case where no convergence result is at hand.

1 Introduction

Domain decomposition algorithms for wave propagation or advection diffusion problems have been designed recently, using two concepts : waveform relaxation algorithms for ordinary differential equations, and absorbing boundary conditions. This approach leads to algorithms which solve the problem iteratively in each subdomain on the whole time interval (with possibly time windows), and exchange informations on the boundary at the end of the time interval. At early stage, Dirichlet transmission conditions where used with overlapping subdomains [4]. Then absorbing boundary conditions were used with or without overlap to improve this exchange of information, thus accelerating enormously the convergence. They were called optimized Schwarz Waveform Relaxation (SWR) algorithms [5][2].

We intend here to investigate the design of such algorithms for the linear Schrödinger equation with a potential, in one space dimension, for two subdomains. We prove rigorously the convergence of the classical one, with overlapping subdomains, exchanging Dirichlet data on the boundaries, for a constant potential.

The key point of the new algorithms is to notice that the convergence in two iterations is obtained when using transparent boundary operators as transmission operators between the subdomains, even in the non-overlapping case. However, they are not available for a general potential, and we prove the convergence of the non overlapping algorithm when using the transparent operators corresponding to the value of the potential on the boundary. The proof uses energy estimates. We also study the possibility of using simpler transmission conditions on the boundary, of complex Robin type. We prove the algorithms to be well-posed and convergent. For overlapping domains, we use Fourier transform in time and exact resolution of the equation in space, and therefore use a constant potential. For non overlapping subdomains, the proof involves energy estimates, and holds for a non constant potential. We also study thoroughly the possibility of optimizing the convergence factor for a constant potential.

We then introduce a finite volume discretization of the algorithm. In the interior, it produces the Crank Nicolson scheme, widely used in the linear and nonlinear computations for the Schrödinger equation, whereas the Robin transmission conditions are naturally taken into account. This idea was first introduced

*LAGA, Institut Galilée, Université Paris XIII, 93430 Villetaneuse, France. halpern@math.univ-paris13.fr

‡Department of Mathematics, Princeton University, Fine Hall, Washington Road, Princeton NJ 08544-1000, USA and C.N.R.S., Mathématiques Appliquées de Bordeaux, Université Bordeaux 1, 351 cours de la Libération, 33405 Talence cedex France. jszeftel@math.princeton.edu. The second author is partially supported by NSF Grant DMS-0504720

in [5] for the wave equation in one dimension. Using a discrete Laplace transform in time, we study the well-posedness and the convergence of the overlapping discrete algorithms, with Dirichlet or Robin exchange of data, for a constant potential. The convergence of the non overlapping Robin SWR is proved with discrete energy estimates.

We finally illustrate and extend the results through numerical simulations, for various types of potential, like constant, barrier, parabolic or linear. We show how slow the convergence is with Dirichlet SWR, and how the optimized SWR improves the convergence. We also show, without proof of convergence, that the best algorithm by far is obtain by using discrete transparent boundary condition designed by Arnold and Ehrhardt precisely for the Crank-Nicolson scheme [1].

Though our results hold only with two subdomains, they clearly extend to any number of subdomains. On another hand due to the the great complexity of the analysis, we restricted ourselves to one dimension in space.

2 Model Problem and Function Spaces

Let V be a real potential in $L^\infty(\mathbb{R})$. We consider here the Schrödinger equation:

$$\mathcal{L}u := i\partial_t u + \partial_{xx}u + Vu = f, \tag{2.1}$$

with the initial condition

$$u(x,0) = u_0(x). \tag{2.2}$$

We first recall some definitions of functional spaces. Let Ω be an open subset of $\mathbb{R}$. The complex Hilbert space $L^2(\Omega)$, is equipped with the hermitian product $(f,g) = \int_\Omega (f\bar{g})(x)dx$ and the norm $||\cdot||$. Then, for r an integer, $H^r(\Omega)$ is the Sobolev space of distributions in $\mathcal{D}'(\Omega)$, whose derivatives of order up to r are in $L^2(\Omega)$. The Sobolev space $H^r(\Omega)$ is equipped with the norm $||v||_{H^r(\Omega)} = (\sum_{|\alpha|\le r} ||D^\alpha v||^2)^{\frac{1}{2}}$. If r is not an integer, the space $H^r(\Omega)$ is defined by interpolation. For the time direction, we will use another characterization. The Sobolev space $H^r(\mathbb{R})$ for real r is also the set of tempered distributions u in $\mathcal{S}'(\mathbb{R})$, whose Fourier transform $\hat{u}$ is such that $(1+\tau^2)^{r/2}\hat{u}$ is in $L^2(\mathbb{R})$. The space $H^r(\mathbb{R})$ is equipped with the norm $\|u\|_{H^r(\mathbb{R})} = \|(1+\tau^2)^{r/2}\hat{u}\|$. Then $H^r(0,T)$ is the set of restrictions of elements in $H^r(\mathbb{R})$, and equipped with the quotient norm $\|u\|_{H^r(0,T)} = \inf \{ \|U\|_{H^r(\mathbb{R})}, U = u \text{ a.e. in } (0,T)\}$. Note that if r is an integer, the second definition is equivalent to the first one, see [6].

Lemma 2.1 (A priori estimates) *If u is a smooth solution of (2.1), (2.2) in $\mathbb{R}\times(0,T)$, then it satisfies for any positive time t the inequalities:*

$$\frac{d}{dt}\|u(\cdot,t)\|^2 \le \|f(\cdot,t)\|^2 + \|u(\cdot,t)\|^2, \tag{2.3}$$

$$\frac{d}{dt}\|\partial_x u(\cdot,t)\|^2 \le \|f(\cdot,t)\|^2 + 2\|\partial_t u(\cdot,t)\|^2 + \|V\|^2_{L^\infty}\|u(\cdot,t)\|^2. \tag{2.4}$$

Proof The first result is obtained by multiplying (2.1) by $\bar{u}$, taking the imaginary part, integrating in space by parts, using the Cauchy-Schwarz inequality on the right-hand side, together with the inequality

$$\alpha\beta \le \frac{\eta}{2}\,\alpha^2 + \frac{1}{2\eta}\,\beta^2, \quad \text{for all } \alpha,\beta \in \mathbb{R}, \text{ and } \eta > 0. \tag{2.5}$$

Remark that the term involving the real potential V vanishes when taking the imaginary part.

The second inequality is obtained by multiplying (2.1) by $\partial_t\bar{u}$, taking the real part, integrating in space by parts, using the Cauchy-Schwarz inequality on the right-hand side, together with (2.5). ■

A weak solution of (2.1) in $\mathbb{R}\times(0,T)$ is defined to be a $u \in \mathcal{D}'(0,T;H^1(\mathbb{R}))$, such that for any v in $H^1(\mathbb{R})$,

$$i\frac{d}{dt}(u,v) - (\partial_x u, \partial_x v) + (Vu,v) = (f,v) \text{ in } \mathcal{D}'(0,T). \tag{2.6}$$

There is an existence theorem in $L^2(0,T;H^1(\mathbb{R}))$ under convenient assumptions on u_0 and f, but the domain decomposition algorithms will require more regularity. We therefore introduce now for any domain $\Omega \subset \mathbb{R}$ the anisotropic Sobolev spaces, defined in [6] as

$$H^{r,s}(\Omega\times(0,T)) = L^2(0,T;H^r(\Omega)) \cap H^s(0,T;L^2(\Omega)). \tag{2.7}$$

If u is in $H^{r,s}(\Omega \times (0,T))$, then for any integer j and k, we have

$$\frac{\partial^j}{\partial x^j}\frac{\partial^k}{\partial t^k}u \in H^{\mu,\nu}(\Omega \times (0,T)), \quad \text{where} \quad \frac{\mu}{r} = \frac{\nu}{s} = 1 - (\frac{j}{r} + \frac{k}{s}). \tag{2.8}$$

Theorem 2.2 (Existence and uniqueness) *If the initial value u_0 is in $H^2(\mathbb{R})$, the real potential V is in $L^\infty(\mathbb{R})$, and the right hand side f is in $H^1(0,T;L^2(\mathbb{R}))$, then there exists a unique solution u of (2.6) in $H^{2,1}(\mathbb{R} \times (0,T))$.*

Proof This classical result is obtained by a Galerkin method, using the *a priori* estimates of Lemma 2.1. We first apply (2.3) to u and $\partial_t u$, with $iu_t(\cdot,0) = f(\cdot,0) - \partial_{xx}u_0 - Vu_0 \in L^2(\mathbb{R})$, then apply (2.4) to u. This gives bounds for u, $\partial_t u$ and $\partial_x u$ in $L^\infty(0,T,L^2(\Omega))$. Equation (2.1) gives $\partial_{xx}u$ in $L^2(0,T,L^2(\Omega))$, which concludes the proof. ■

At the interfaces between subdomains, the Schwarz waveform relaxation algorithm will need traces of the subdomain approximations to the solution. We therefore introduce the space $V^{r,s}(\Omega \times (0,T))$ of traces of functions in $H^{r,s}(\Omega \times (0,T))$ for the half-line $\Omega = \mathbb{R}_-$ (and similarly for $\Omega = \mathbb{R}_+$). Denoting by f_k the trace of the k-th derivative in time at $t=0$, and by g_j the trace of the j-th derivative in space on the boundary $\{0\} \times (0,T)$, the trace space $V^{r,s}(\Omega \times (0,T))$ is defined for $T = +\infty$ by

$$\begin{aligned} V^{r,s}(\Omega \times (0,T)) := \Big\{ \big((f_k)_{k<s-\frac{1}{2}}, (g_j)_{j<r-\frac{1}{2}}\big) \in \textstyle\prod_{k<s-\frac{1}{2}} H^{p_k}(\Omega) \times \prod_{j<r-\frac{1}{2}} H^{\mu_j}(0,T), \\ p_k = \tfrac{r}{s}(s-k-\tfrac{1}{2}), \quad \mu_j = \tfrac{s}{r}(r-j-\tfrac{1}{2}), \\ \partial_t^k g_j(0) = \partial_x^j f_k(0), \quad \text{if } \tfrac{j}{r} + \tfrac{k}{s} < 1 - \tfrac{1}{2}(\tfrac{1}{r} + \tfrac{1}{s}), \\ \textstyle\int_0^\infty |\partial_x^j f_k(\sigma^s) - \partial_t^k g_j(\sigma^r)|^2 \frac{d\sigma}{\sigma} < \infty, \quad \text{if } \tfrac{j}{r} + \tfrac{k}{s} = 1 - \tfrac{1}{2}(\tfrac{1}{r} + \tfrac{1}{s}) \Big\}. \end{aligned} \tag{2.9}$$

Theorem 2.3 *For positive real numbers r and s such that $1 - \frac{1}{2}(\frac{1}{r} + \frac{1}{s}) > 0$, the trace map*

$$u \mapsto \Big(\big(\frac{\partial^k u}{\partial t^k}(x,0)\big)_{k<s-\frac{1}{2}}, \big(\frac{\partial^j u}{\partial x^j}(0,t)\big)_{j<r-\frac{1}{2}} \Big) \tag{2.10}$$

is defined and continuous from $H^{r,s}(\Omega \times (0,T))$ onto $V^{r,s}(\Omega \times (0,T))$.

Proof The proof can be found in [6]. ■

3 Classical Schwarz Waveform Relaxation

We decompose the spatial domain $\Omega = \mathbb{R}$ into two overlapping subdomains $\Omega_1 = (-\infty, L)$ and $\Omega_2 = (0,\infty)$, with $L > 0$. The overlapping Schwarz waveform relaxation algorithm consists in solving iteratively subproblems on $\Omega_1 \times (0,T)$ and $\Omega_2 \times (0,T)$ using as a boundary condition at the interfaces $x=0$ and $x=L$ the values obtained from the previous iteration. The algorithm is thus for iteration index $k = 1, 2, \ldots$ given by

$$\begin{cases} \mathcal{L}u_1^k = f \text{ in } \Omega_1 \times (0,T), \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1, \\ u_1^k(L,\cdot) = u_2^{k-1}(L,\cdot) \text{ in } (0,T), \end{cases} \qquad \begin{cases} \mathcal{L}u_2^k = f \text{ in } \Omega_2 \times (0,T), \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2, \\ u_2^k(0,\cdot) = u_1^{k-1}(0,\cdot) \text{ in } (0,T). \end{cases} \tag{3.1}$$

For the initial guess, we only need to provide boundary data, and the convention will be that

$$g_L = u_2^0(L,\cdot), \quad g_0 = u_1^0(0,\cdot).$$

We first study the well posedness of algorithm (3.1), and then analyze its convergence properties.

3.1 Well Posedness of the Algorithm

Without loss of generality, we consider the subdomain problem on Ω_1 only,

$$\begin{cases} \mathcal{L}v = f \text{ in } \Omega_1 \times (0,T), \\ v(\cdot,0) = u_0 \text{ in } \Omega_1, \\ v(L,\cdot) = g \text{ in } (0,T). \end{cases} \tag{3.2}$$

Proposition 3.1 *Let V be a real constant. If $f \in H^1(0,T;L^2(\Omega_1))$, $u_0 \in H^2(\Omega_1)$ and $g \in H^{\frac{3}{4}}(0,T)$, and if the compatibility condition*

$$u_0(L) = g(0) \tag{3.3}$$

is satisfied, then problem (3.2) has a unique solution v in $H^{1,0}(\Omega_1 \times (0,T))$. Furthermore $v(0,\cdot)$ is in $H^{\frac{3}{4}}(0,T)$, and the following compatibility formula is valid:

$$\lim_{t\to 0_+} v(0,t) = u_0(0). \tag{3.4}$$

Remark 3.2 *By the Sobolev Embedding Theorem [6], u_0 is continuous on $\overline{\Omega}_1$, $v(0,\cdot)$ and g are continuous on $[0,T]$, which gives a classical meaning to equalities (3.3) and (3.4).*

Proof We start with the uniqueness result. Since the problem is linear, we consider vanishing data. Multiplying the equation by $\bar{v}$, taking the imaginary part and integrating by parts in space yields

$$\frac{d}{dt}\|v\|^2 = 0,$$

and thus $v = 0$. As for the existence result, we shall use Fourier transform in time. We define $w = v - u$, where u is the solution of (2.1),(2.2) in $\mathbb{R} \times (0,T)$. w is a solution of the Schrödinger equation, with homogeneous right-hand side and initial value, and boundary data $w(L,\cdot) = h$ in $(0,T)$, where $h = g - u(L,\cdot)$. By Trace Theorem 2.3, since u is in $H^{2,1}(\Omega \times (0,T))$, $u(L,\cdot)$ is in $H^{\frac{3}{4}}(0,T)$, and so is h. We now show an existence result for w, or rather for $z = we^{-t}$, solution of the intermediate problem

$$\begin{cases} i\partial_t z + iz + \partial_{xx} z + Vz = 0 \text{ in } \Omega_1 \times (0,T), \\ z(\cdot,0) = 0 \text{ in } \Omega_1, \\ z(L,\cdot) = h_1 \text{ in } (0,T), \end{cases} \tag{3.5}$$

with $h_1 = he^{-t}$. By the compatibility condition (3.3), $h_1(0) = h(0) = g(0) - u(L,0) = g(0) - u_0(L) = 0$. Hence we can extend h_1 in $H^{3/4}(\mathbb{R})$ by H_1 vanishing on $(-\infty,0)$. We extend problem (3.5) in time on $\mathbb{R}$, and the solution coïncides with z on $(0,T)$. Therefore we still call it z. For ϕ in $L^2(\mathbb{R})$, the Fourier transform of ϕ is given by

$$\mathcal{F}\phi(\tau) = \widehat{\phi}(\tau) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \phi(t)\, e^{-i\tau t} dt.$$

We now Fourier transform in time the first equation in (3.5), and get

$$(i - \tau + V)\hat{z} + \partial_{xx}\hat{z} = 0,$$

from which we deduce the exact formula

$$\hat{z}(x,\tau) = \widehat{H}_1(\tau) e^{-(\tau - V - i)^{1/2}(L-x)},\ x < L. \tag{3.6}$$

$(\tau - V - i)^{1/2}$ is the unique analytic determination of the square root of $\tau - V - i$ with positive real part:

$$(\tau - V - i)^{1/2} = \sqrt{\frac{\tau - V + \sqrt{(\tau - V)^2 + 1}}{2}} - i\sqrt{\frac{-\tau + V + \sqrt{(\tau - V)^2 + 1}}{2}}. \tag{3.7}$$

The norm of z in $L^2(\Omega_1 \times \mathbb{R})$ is now given by the Parseval identity,

$$\|z\|_{L^2(\Omega_1\times\mathbb{R})} = \|\hat{z}\|_{L^2(\Omega_1\times\mathbb{R})} = \left\| \frac{\widehat{H}_1(\tau)}{\sqrt{2\mathcal{R}e\,(\tau - V - i)^{1/2}}} \right\|_{L^2(\mathbb{R})}.$$

When $\tau \to \pm\infty$, the real part of $(\tau - V - i)^{1/2}$ has the following behavior:

$$\mathcal{R}e\,(\tau - V - i)^{1/2} \approx \begin{cases} \sqrt{\tau}, & \tau > 0, \\ \dfrac{1}{2\sqrt{-\tau}}, & \tau < 0, \end{cases} \approx \begin{cases} (1+\tau^2)^{1/4}, & \tau > 0, \\ \dfrac{1}{2}(1+\tau^2)^{-1/4}, & \tau < 0. \end{cases} \tag{3.8}$$

Therefore, we have $\|z\|_{L^2(\Omega_1\times\mathbb{R})} \le \|H_1\|_{H^{1/4}(\mathbb{R})}$, and taking the infimum on all the extensions H_1 of h_1 we obtain

$$\|z\|_{L^2(0,T,L^2(\Omega_1))} \le \|z\|_{L^2(\Omega_1\times\mathbb{R})} \le \|h_1\|_{H^{1/4}(\mathbb{R})}\,. \tag{3.9}$$

We now evaluate $\partial_x z$ the same way:

$$\|\partial_x z\|_{L^2(\Omega_1\times\mathbb{R})} = \left\| \frac{(\tau - V - i)^{1/2}}{\sqrt{2\mathcal{R}e\,(\tau - V - i)^{1/2}}}\widehat{H}_1(\tau)\right\|_{L^2(\mathbb{R})}.$$

Since

$$\left|\frac{(\tau - V - i)^{1/2}}{\sqrt{2\mathcal{R}e\,(\tau - V - i)^{1/2}}}\right| = \frac{(1+(\tau-V)^2)^{1/4}}{|\sqrt{2\mathcal{R}e\,(\tau - V - i)^{1/2}}|} \lesssim (1+\tau^2)^{3/8},$$

we get the upper bound

$$\|\partial_x z\|_{L^\infty(0,T,L^2(\Omega_1))} \le \|h_1\|_{H^{3/4}(\mathbb{R})}\,.$$

Therefore (3.6) defines the Fourier transform of a function z in $H^{1,0}(\Omega_1\times(0,T))$, solution of (3.5). This proves the existence of w, and hence of v, in $H^{1,0}(\Omega_1\times(0,T))$. We now prove that $z(0,.)$ is in $H^{3/4}(0,T)$. Due to (3.6), we have

$$\hat{z}(0,\tau) = \widehat{H}_1(\tau)e^{-(\tau-V-i)^{1/2}L}, \tag{3.10}$$

and $|\hat{z}(0,\tau)| \le |\widehat{H}_1(\tau)|$. Since h_1 is in $H^{3/4}(0,T)$, so is $z(0,\cdot)$, and

$$\|z(0,\cdot)\|_{H^{3/4}(0,T)} \le \|H_1\|_{H^{3/4}(0,T)}.$$

As for the compatibility relation, since H_1 is supported in $\mathbb{R}_+$, $\widehat{H}_1$ is analytic in the half-plane $\mathcal{I}m\,\tau < 0$, and by (3.10) and Paley-Wiener Theorem (see e.g. [9]), $z(0,\cdot)$ is supported in $\mathbb{R}_+$. Since we just proved that $z(0,\cdot)$ is in $H^{3/4}(0,T)$, and since $H^{3/4}(0,T) \subset \mathcal{C}([0,T])$ by the Sobolev Embedding Theorem [6], we have $\lim_{t\to 0_+} z(0,t) = 0$. By the definition of z, it implies that $\lim_{t\to 0_+} v(0,t) = \lim_{t\to 0_+} u(0,t)$. Since u is in $H^{2,1}(\Omega\times(0,T))$, by Trace Theorem 2.3, it satisfies the compatibility conditions $\lim_{t\to 0_+} u(0,t) = u_0(0)$, which establish relation (3.4) and concludes the proof of the proposition. ■

The preceding result ensures that the subdomain problems are well posed in the classical algorithm, provided the initial and boundary conditions satisfy the compatibility condition (3.3) for each iteration step, as stated in the next Theorem.

Theorem 3.3 *Let g_L and g_0 be given in $H^{\frac{3}{4}}(0,T)$, such that $g_L(0) = u_0(L)$ and $g_0(0) = u_0(0)$. Let V be a real constant. Then (3.1) defines a sequence of iterates (u_1^k, u_2^k) in $H^{1,0}(\Omega_1\times(0,T))\times H^{1,0}(\Omega_2\times(0,T))$, with $u_1^k(0,\cdot)$ and $u_2^k(L,\cdot)$ in $H^{\frac{3}{4}}(0,T)$, with the compatibility relations*

$$\lim_{t\to 0_+} u_1^k(0,t) = u_0(0),\ \ \lim_{t\to 0_+} u_2^k(L,t) = u_0(L).$$

Proof The proof is done by induction. Let g_L and g_0 be given in $H^{\frac{3}{4}}(0,T)$, such that $g_L(0) = u_0(L)$ and $g_0(0) = u_0(0)$. By Proposition 3.1, this defines a unique first iterate (u_1^1, u_2^1) in $H^{1,0}(\Omega_1\times(0,T))\times H^{1,0}(\Omega_2\times(0,T))$, $u_1^1(0,\cdot)$ in $H^{\frac{3}{4}}(0,T)$ and $u_2^1(L,\cdot)$ in $H^{\frac{3}{4}}(0,T)$. Furthermore we have the compatibility relations $\lim_{t\to 0_+} u_1^1(0,t) = u_0(0)$ and $\lim_{t\to 0_+} u_2^1(L,t) = u_0(L)$, which in turn enables to define a second iterate (u_1^2, u_2^2), and so on. ■

3.2 Convergence of the Algorithm

By linearity, the error between the solution u and the iterates u_j^k, $j = 1,2$, of algorithm (3.1) satisfies a homogeneous Schrödinger equation with homogeneous initial condition. We therefore study in the sequel the homogeneous problem with data on the interfaces only. Let h_L and h_0 be given in $H^{\frac{3}{4}}(0,T)$ with $h_L(0) = 0$ and $h_0(0) = 0$, to satisfy the compatibility conditions, and let (e_1, e_2) be the solution in $H^{2,1}(\Omega_1\times(0,T))\times H^{2,1}(\Omega_2\times(0,T))$ of the equations

$$\begin{cases} \mathcal{L}e_1 = 0 \text{ in } \Omega_1\times(0,T), \\ e_1(\cdot,0) = 0 \text{ in } \Omega_1, \\ e_1(L,\cdot) = h_L \text{ in } (0,T), \end{cases} \qquad \begin{cases} \mathcal{L}e_2 = 0 \text{ in } \Omega_2\times(0,T), \\ e_2(\cdot,0) = 0 \text{ in } \Omega_2, \\ e_2(0,\cdot) = h_0 \text{ in } (0,T). \end{cases} \tag{3.11}$$

Our analysis is based again on the Fourier transform in time. We define for $r > \frac{1}{2}$ the one-sided space

$$_0H^r(0,T) = \{\phi \in H^r(0,T), \phi(0) = 0\},$$

equipped with the norm

$$\|\phi\|_{_0H^r(0,T)} = \inf \{ \|\Phi\|_{H^r(\mathbb{R})}, \Phi = \phi \text{ a.e. in } (0,T), \Phi = 0 \text{ a.e. in } (-\infty,0)\}.$$

Lemma 3.4 *Suppose $L \geq 0$. Let V be a real constant. The map $\mathcal{G}_D$ associated with the equations (3.11),*

$$\mathcal{G}_D : (e^{-t}h_L, e^{-t}h_0) \mapsto (e^{-t}e_2(L,\cdot), e^{-t}e_1(0,\cdot)), \tag{3.12}$$

is a contraction on $(_0H^{\frac{3}{4}}(0,T))^2$. The local convergence factor is defined as

$$\theta_D(\tau, L) = e^{-(\tau-V-i)^{1/2}L}. \tag{3.13}$$

Moreover, if $L > 0$ and if there is $\tau_{max} > 0$ such that $\widehat{e^{-t}h_L}$ and $\widehat{e^{-t}h_0}$ vanish outside $[-\tau_{max}, +\infty)$, then $\mathcal{G}_D$ is a strict contraction: defining the maximal convergence factor as

$$\Theta_D(\tau_{max}, L) = exp\left[-\left(\frac{-\tau_{max} + V + \sqrt{1 + (\tau_{max} - V)^2}}{2}\right)^{1/2} L\right] < 1, \tag{3.14}$$

one has

$$\|\mathcal{G}_D(e^{-t}h_L, e^{-t}h_0)\|_{(H^{\frac{3}{4}}(0,T))^2} \leq \Theta_D(\tau_{max}, L)\|(e^{-t}h_L, e^{-t}h_0)\|_{(H^{\frac{3}{4}}(0,T))^2}. \tag{3.15}$$

Remark 3.5 *The assumptions on the supports of the data will be satisfied in the numerical computations since the maximal numerical frequency is $\tau_{max} = \pi/\Delta t$.*

Proof By the existence result in Proposition 3.1, $\mathcal{G}_D$ maps $(_0H^{\frac{3}{4}}(0,T))^2$ into itself. We now multiply h_L and h_0 in $H^{\frac{3}{4}}(0,T)$ by e^{-t}, extend the result by H_L and H_0 in $H^{\frac{3}{4}}(\mathbb{R})$, vanishing on $(-\infty, 0)$, extend (3.11) in time on $\mathbb{R}$, define $E_j = e_j e^{-t}$, and Fourier transform the resulting equation in time as in the proof of Proposition 3.1. We find again

$$\hat{E}_1 = \widehat{H}_L(\tau)e^{-(\tau-V-i)^{1/2}(L-x)}, \qquad \hat{E}_2 = \widehat{H}_0(\tau)e^{-(\tau-V-i)^{1/2}x}, \tag{3.16}$$

which gives $\mathcal{F}(\mathcal{G}_D(e^{-t}h_L, e^{-t}h_0))(\tau) = \theta_D(\tau, L)(\mathcal{F}(e^{-t}h_0)(\tau), \mathcal{F}(e^{-t}h_L)(\tau))$, and

$$|\mathcal{F}(\mathcal{G}_D(e^{-t}h_L, e^{-t}h_0))(\tau)| \leq \sup_{\tau\in[-\tau_{max},+\infty)} |\theta_D(\tau, L)||(\mathcal{F}(e^{-t}h_0)(\tau), \mathcal{F}(e^{-t}h_L)(\tau))|.$$

We have by (3.7)

$$\sup_{\tau\in[-\tau_{max},+\infty)} |\theta_D(\tau, L)| = |\theta_D(-\tau_{max}, L)| = \Theta_D(\tau_{max}, L),$$

which finally yields (3.15). ∎

We now prove the convergence of the overlapping Schwarz waveform relaxation algorithm.

Theorem 3.6 *Let an initial guess (g_0, g_L) in $(H^{\frac{3}{4}}(0,T))^2$ such that $g_0(0) = u_0(0)$ and $g_L(0) = u_0(L)$. Let V be a real constant. Suppose there is a $\tau_{max} > 0$ such that $\widehat{e^{-t}h_L}$ and $\widehat{e^{-t}h_0}$ vanish outside $[-\tau_{max}, +\infty)$, with $h_0 = g_0 - u(0,\cdot)$ and $h_L = g_L - u(L,\cdot)$. Then the iterates (u_1^k, u_2^k) of algorithm (3.1) converge in $L^2(\Omega_1 \times (0,T)) \times L^2(\Omega_2 \times (0,T))$ to the solution of (2.1), (2.2).*

Proof The errors $e_j^k = u_j^k - u$, $j = 1, 2$, satisfy for $k \geq 2$ the equations

$$\begin{cases} \mathcal{L}e_1^k = 0 \text{ in } \Omega_1 \times (0,T), \\ e_1^k(\cdot, 0) = 0 \text{ in } \Omega_1, \\ e_1^k(L, \cdot) = e_2^{k-1}(L, \cdot) \text{ in } (0,T), \end{cases} \qquad \begin{cases} \mathcal{L}e_2^k = 0 \text{ in } \Omega_2 \times (0,T), \\ e_2^k(\cdot, 0) = 0 \text{ in } \Omega_2, \\ e_2^k(0, \cdot) = e_1^{k-1}(0, \cdot) \text{ in } (0,T). \end{cases} \tag{3.17}$$

For positive k, we introduce the interface functions $h_L^k = e_2^k(L,\cdot)$ and $h_0^k = e_1^k(0,\cdot)$ and denote by $h_0^0 = h_0$ and $h_L^0 = h_L$. Using Lemma 3.4, we obtain first by formula (3.6) and induction that if $\widehat{e^{-t}h_L}$ and $\widehat{e^{-t}h_0}$ vanish outside $[-\tau_{max}, +\infty)$, then for any k, $\widehat{e^{-t}h_L^k}$ and $\widehat{e^{-t}h_0^k}$ vanish outside $[-\tau_{max}, +\infty)$ as well. Second, introducing the map $\mathcal{G}_D$ given in (3.12), we have

$$(e^{-t}h_L^{k+1}, e^{-t}h_0^{k+1}) = \mathcal{G}_D(e^{-t}h_0^k, e^{-t}h_L^k) = \mathcal{G}_D^2(e^{-t}h_L^{k-1}, e^{-t}h_0^{k-1}),$$

which proves that

$$(e^{-t}h_L^{2k}, e^{-t}h_0^{2k}) = \mathcal{G}_D^{2k}(e^{-t}h_L^0, e^{-t}h_0^0), \tag{3.18}$$

$$(e^{-t}h_L^{2k+1}, e^{-t}h_0^{2k+1}) = \mathcal{G}_D^{2k+1}(e^{-t}h_0^0, e^{-t}h_L^0) \tag{3.19}$$

and thus by Lemma 3.4

$$\|(e^{-t}h_L^k, e^{-t}h_0^k)\|_{(H^{\frac{3}{4}}(0,T))^2} \leq \Theta_D(\tau_{max}, L)^k \|(e^{-t}h_L^0, e^{-t}h_0^0)\|_{(H^{\frac{3}{4}}(0,T))^2},$$

with $\Theta_D(\tau_{max}, L)$ given in (3.14). By estimate (3.9), we deduce that

$$\|e^{-t}e_j^k\|_{L^2(\Omega_j\times(0,T))} \leq \Theta_D(\tau_{max}, L)^{k-1} \|(e^{-t}h_L^0, e^{-t}h_0^0)\|_{(H^{\frac{3}{4}}(0,T))^2},$$

and therefore

$$\begin{aligned}\|e_j^k\|_{L^2(\Omega_j\times(0,T))} &\leq e^T \|e^{-t}e_j^k\|_{L^2(\Omega_j\times(0,T))} \\ &\leq e^T \Theta_D(\tau_{max}, L)^{k-1} \|(e^{-t}h_L^0, e^{-t}h_0^0)\|_{(H^{\frac{3}{4}}(0,T))^2}\end{aligned}$$

which yields

$$\|e_j^k\|_{L^2(\Omega_j\times(0,T))} \leq e^T \Theta_D(\tau_{max}, L)^{k-1} \|(h_L^0, h_0^0)\|_{(H^{\frac{3}{4}}(0,T))^2}. \tag{3.20}$$

■

Theorem 3.6 shows that the overlapping Schwarz waveform relaxation algorithm converges, that the convergence factor $\Theta_D(\tau_{max}, L)$ is at least linear, and independent of the length of the time interval. It does however depend on the overlap L, as all overlapping Schwarz methods do, but also on the smaller negative frequency $-\tau_{max}$. It tends to 1 when L tends to 0, and also when τ_{max} tends to infinity, which differs from what happens for wave equations [5] or parabolic equations [2].

4 Optimal Schwarz Waveform Relaxation Algorithm

We proved in previous works that the best choice for the transmission conditions would be to use transparent boundary operators in the sense we describe now. Let $\mathcal{S}_1$ and $\mathcal{S}_2$ be linear operators acting only in time. We introduce the algorithm

$$\begin{cases} \mathcal{L}u_1^k = f \text{ in } \Omega_1 \times (0,T), \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1, \\ (\partial_x + \mathcal{S}_1)u_1^k(L,\cdot) = (\partial_x + \mathcal{S}_1)u_2^{k-1}(L,\cdot) \text{ in } (0,T), \end{cases} \quad \begin{cases} \mathcal{L}u_2^k = f \text{ in } \Omega_2 \times (0,T), \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2, \\ (\partial_x + \mathcal{S}_2)u_2^k(0,\cdot) = (\partial_x + \mathcal{S}_2)u_1^{k-1}(0,\cdot) \text{ in } (0,T). \end{cases} \tag{4.1}$$

We define the symbol σ_j of $\mathcal{S}_j(\partial_t)$ by $\sigma_j(\tau) := \mathcal{S}_j(i\tau)$.

Theorem 4.1 *Let V be a real constant. Algorithm (4.1) converges to the solution u of (2.1) in two iterations for all initial guesses u_1^0 and u_2^0, independently of the size of the overlap $L \geq 0$, if and only if the operators $\mathcal{S}_1$ and $\mathcal{S}_2$ have the corresponding symbols*

$$\sigma_1 = (\tau - V)^{1/2}, \quad \sigma_2 = -(\tau - V)^{1/2} \tag{4.2}$$

with

$$(\tau - V)^{1/2} = \begin{cases} \sqrt{\tau - V} \text{ if } \tau \geq V, \\ -i\sqrt{-\tau + V} \text{ if } \tau < V. \end{cases} \tag{4.3}$$

Proof Using the Fourier transform with parameter τ as before, and the equations for the error with vanishing data, we find the errors to be given by

$$\widehat{e_1^k}(x,\tau) = \alpha^k(\tau)e^{-(\tau-V)^{1/2}(L-x)}, \quad \widehat{e_2^k}(x,\tau) = \beta^k(\tau)e^{-(\tau-V)^{1/2}x}, \quad k \geq 1. \tag{4.4}$$

With the general transmission conditions in (4.1), we obtain for $k \geq 1$,

$$\begin{aligned} \alpha^k((\tau-V)^{1/2}+\sigma_1) &= \beta^{k-1}(-(\tau-V)^{1/2}+\sigma_1)e^{-(\tau-V)^{1/2}L}, \\ \beta^k(-(\tau-V)^{1/2}+\sigma_2) &= \alpha^{k-1}((\tau-V)^{1/2}+\sigma_2)e^{-(\tau-V)^{1/2}L}. \end{aligned} \tag{4.5}$$

Now for an arbitrary initial guess u_1^0 and u_2^0, the coefficients α^1 and β^1 will in general not vanish. Since $-(\tau-V)^{1/2}+\sigma_1 = (\tau-V)^{1/2}+\sigma_2 = 0$ implies $(\tau-V)^{1/2}+\sigma_1 \neq 0$ and $-(\tau-V)^{1/2}+\sigma_2 \neq 0$, we obtain from (4.5) that α^2 and β^2 are identically zero if and only if $-(\tau-V)^{1/2}+\sigma_1 = (\tau-V)^{1/2}+\sigma_2 = 0$. ■

For variable potentials, the optimal operators are in general not at hand. We present here and will compare two approximations of those. The first one is to use a "frozen coefficients" variant of these operators. The second one is to replace them by a constant, obtaining "Robin type" transmission conditions, and to optimize them by minimizing the convergence factor in the constant case.

5 The Quasi-optimal Algorithm

We use as transmission operators the optimal operators for the constant potential equal to the value of V on the interface. The quasi-optimal algorithm is thus for iteration index $k = 1, 2, \ldots$ given by

$$\begin{cases} \mathcal{L}u_1^k = f \text{ in } \Omega_1 \times (0,T), \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1, \\ (\partial_x + \sqrt{-i\partial_t - V(L)})u_1^k(L,\cdot) \\ \quad = (\partial_x + \sqrt{-i\partial_t - V(L)})u_2^{k-1}(L,\cdot) \text{ in } (0,T), \end{cases} \qquad \begin{cases} \mathcal{L}u_2^k = f \text{ in } \Omega_2 \times (0,T), \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2, \\ (\partial_x - \sqrt{-i\partial_t - V(0)})u_2^k(0,\cdot) \\ \quad = (\partial_x - \sqrt{-i\partial_t - V(0)})u_1^{k-1}(0,\cdot) \text{ in } (0,T) \end{cases} \tag{5.1}$$

where $\sqrt{-i\partial_t - V(x)}$ is the operator acting only in time with symbol:

$$(\tau - V(x))^{1/2} = \begin{cases} \sqrt{\tau - V(x)} \text{ if } \tau \geq V(x), \\ -i\sqrt{-\tau + V(x)} \text{ if } \tau < V(x). \end{cases} \tag{5.2}$$

Though being not differential, this operator is still easy to use numerically [1].

We call the algorithm (5.1) quasi optimal, in the sense that it is optimal for a constant potential. It is initialized by using only boundary data, therefore we define formally

$$g_L := (\partial_x + \sqrt{-i\partial_t - V(L)})u_2^0(L,\cdot), \quad g_0 := (\partial_x - \sqrt{-i\partial_t - V(0)})u_1^0(0,\cdot).$$

5.1 Well-posedness of the algorithm

For a constant potential, the proof of well-posedness relies on Fourier transform in time and exact computation of the solution as in (3.6). We do not have a proof of well-posedness in the case where V is a variable potential. On the other hand, we are able to prove the convergence of the non overlapping algorithm in that case as shown in the next section.

5.2 Convergence of the Non-Overlapping Algorithm for a non constant potential V

We prove the convergence of the quasi-optimal algorithm when there is no overlap ,*i.e.* $L = 0$, and when $T = +\infty$.

Theorem 5.1 *Let $L = 0$ and $T = +\infty$. Let V and V' belong to $L^\infty(\mathbb{R})$. Then the iterates (u_1^k, u_2^k) of algorithm (5.1) converge in*

$$(H^{1/4}(0,T,L^2(\Omega_1)) \cap H^{-1/4}(0,T,H^1(\Omega_1))) \times (H^{1/4}(0,T,L^2(\Omega_2)) \cap H^{-1/4}(0,T,H^1(\Omega_2)))$$

to the solution of (2.1), (2.2).

Proof The errors $e_j^k = u_j^k - u$, $j = 1,2$, satisfy for $k \geq 2$ the equations

$$\begin{cases} \mathcal{L}e_1^k = 0 \text{ in } \Omega_1 \times (0,+\infty), \\ e_1^k(\cdot,0) = 0 \text{ in } \Omega_1, \\ (\partial_x + \sqrt{-i\partial_t - V(0)})e_1^k(0,\cdot) \\ \ = (\partial_x + \sqrt{-i\partial_t - V(0)})e_2^{k-1}(0,\cdot) \text{ in } (0,+\infty), \end{cases} \qquad \begin{cases} \mathcal{L}e_2^k = 0 \text{ in } \Omega_2 \times (0,+\infty), \\ e_2^k(\cdot,0) = 0 \text{ in } \Omega_2, \\ (\partial_x - \sqrt{-i\partial_t - V(0)})e_2^k(0,\cdot) \\ \ = (\partial_x - \sqrt{-i\partial_t - V(0)})e_1^{k-1}(0,\cdot) \text{ in } (0,+\infty). \end{cases} \tag{5.3}$$

We introduce $\eta > 0$ satisfying

$$\eta \geq \|V'\|_{L^\infty(\mathbb{R})}^{2/3}. \tag{5.4}$$

Let E_j^k be the extension of $e^{-\eta t}e_j^k$ to $\mathbb{R} \times \Omega_j$ vanishing on $(-\infty,0) \times \Omega_j$. E_j^k, $j = 1,2$, satisfy for $k \geq 2$ the equations

$$\begin{cases} (i\partial_t + \partial_{xx} + V + i\eta)E_1^k = 0 \text{ in } \Omega_1 \times \mathbb{R}, \\ (\partial_x + \sqrt{-i\partial_t - V(0) - i\eta})E_1^k(0,\cdot) \\ \ = (\partial_x + \sqrt{-i\partial_t - V(0) - i\eta})E_2^{k-1}(0,\cdot) \text{ in } \mathbb{R}, \end{cases} \qquad \begin{cases} (i\partial_t + \partial_{xx} + V + i\eta)E_2^k = 0 \text{ in } \Omega_2 \times \mathbb{R}, \\ (\partial_x - \sqrt{-i\partial_t - V(0) - i\eta})E_2^k(0,\cdot) \\ \ = (\partial_x - \sqrt{-i\partial_t - V(0) - i\eta})E_1^{k-1}(0,\cdot) \text{ in } \mathbb{R}, \end{cases} \tag{5.5}$$

where we have used the fact that $e_j^k(\cdot,0) = 0$ in Ω_j, $j = 1,2$, and the identity

$$e^{-\eta t}\sqrt{-i\partial_t - V(0)}e^{\eta t} = \sqrt{-i\partial_t - V(0) - i\eta}.$$

Here, $\sqrt{-i\partial_t - V(x) - i\eta}$ is the operator acting only in time with symbol:

$$(\tau - V(x) - i\eta)^{1/2} \tag{5.6}$$

where $(\tau - V(x) - i\eta)^{1/2}$ is the unique analytic determination of the square root with positive real part.

Multiplying the equation of E_1^k in (5.5) by $\overline{\sqrt{-i\partial_t - V(x) - i\eta}E_1^k}$, taking the real part, integrating in time, and integrating by parts in space yields

$$\begin{aligned} &\mathcal{R}e \int_{\mathbb{R}}\int_{-\infty}^{0} (-i\partial_t - V(x) - i\eta)E_1^k \overline{\sqrt{-i\partial_t - V(x) - i\eta}E_1^k} dxdt \\ &+\mathcal{R}e \int_{\mathbb{R}}\int_{-\infty}^{0} \sqrt{-i\partial_t - V(x) - i\eta}\partial_x E_1^k \overline{\partial_x E_1^k} dxdt \\ &-\mathcal{R}e \int_{\mathbb{R}} \partial_x E_1^k(0,.)\overline{\sqrt{-i\partial_t - V(0) - i\eta}E_1^k(0,.)}dt \\ &= \frac{1}{2}\mathcal{R}e \int_{\mathbb{R}}\int_{-\infty}^{0} V'(x)\partial_x E_1^k \overline{\sqrt{-i\partial_t - V(x) - i\eta}^{-1} E_1^k} dxdt \end{aligned} \tag{5.7}$$

where we have used the identity

$$\partial_x(\sqrt{-i\partial_t - V(x) - i\eta}\, w) = \sqrt{-i\partial_t - V(x) - i\eta}\, \partial_x w - \frac{V'(x)}{2}\sqrt{-i\partial_t - V(x) - i\eta}^{-1} w.$$

By using Plancherel in time and

$$\mathcal{R}e\,(a\bar{b}) = \frac{1}{4}(|a+b|^2 - |a-b|^2)$$

we obtain:

$$\begin{aligned} &\int_{\mathbb{R}}\int_{-\infty}^{0} \mathcal{R}e\,(\sqrt{\tau - V(x) - i\eta})(\eta^2 + (\tau - V(x))^2)^{1/2}|\widehat{E_1^k}(\tau,x)|^2 dxd\tau \\ &+ \int_{\mathbb{R}}\int_{-\infty}^{0} \mathcal{R}e\,(\sqrt{\tau - V(x) - i\eta})|\widehat{\partial_x E_1^k}(\tau,x)|^2 dxd\tau \\ &+\frac{1}{4}\int_{\mathbb{R}} |\partial_x E_1^k(0,.) - \sqrt{-i\partial_t - V(0) - i\eta}E_1^k(0,.)|^2 dt \\ &\leq \frac{1}{4}\int_{\mathbb{R}} |\partial_x E_1^k(0,.) + \sqrt{-i\partial_t - V(0) - i\eta}E_1^k(0,.)|^2 dt \\ &+\frac{\|V'\|_{L^\infty}}{2}\int_{\mathbb{R}}\int_{-\infty}^{0} (\eta^2 + (\tau - V(x))^2)^{-\frac{1}{4}}|\widehat{\partial_x E_1^k}(\tau,x)||\widehat{E_1^k}(\tau,x)|dxd\tau. \end{aligned} \tag{5.8}$$

We have

$$\begin{aligned}&\frac{\|V'\|_{L^\infty}}{2}\int_{\mathbb{R}}\int_{-\infty}^0(\eta^2+(\tau-V(x))^2)^{-\frac14}|\widehat{\partial_x E_1^k}(\tau,x)||\widehat{E_1^k}(\tau,x)|dxd\tau\\&\le\frac12\int_{\mathbb{R}}\int_{-\infty}^0\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})|\widehat{\partial_x E_1^k}(\tau,x)|^2dxd\tau\\&+\frac{\|V'\|^2_{L^\infty}}{8}\int_{\mathbb{R}}\int_{-\infty}^0\frac{|\widehat{E_1^k}(\tau,x)|^2}{\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})(\eta^2+(\tau-V(x))^2)^{\frac12}}dxd\tau.\end{aligned}\tag{5.9}$$

Now as

$$\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})=\left(\frac{\tau-V(x)+\sqrt{(\tau-V(x))^2+\eta^2}}{2}\right)^{1/2}$$

we get

$$\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})\ge\frac{\eta}{2(\eta^2+(\tau-V(x))^2)^{1/4}}\tag{5.10}$$

which in turn yields

$$\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})^2(\eta^2+(\tau-V(x))^2)\ge\frac{\eta^2(\eta^2+(\tau-V(x))^2)^{1/2}}{4}\ge\frac{\eta^3}{4}.$$

Therefore:

$$\begin{aligned}&\frac{\|V'\|^2_{L^\infty}}{8}\frac{1}{\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})(\eta^2+(\tau-V(x))^2)^{\frac12}}\\&\le\frac{\|V'\|^2_{L^\infty}}{2\eta^3}\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})(\eta^2+(\tau-V(x))^2)^{\frac12}\\&\le\frac12\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})(\eta^2+(\tau-V(x))^2)^{\frac12}\end{aligned}\tag{5.11}$$

where we have used (5.4) to get the last inequality. Thus, using (5.8), (5.9) and (5.11) we obtain:

$$\begin{aligned}&\int_{\mathbb{R}}\int_{-\infty}^0\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})(\eta^2+(\tau-V(x))^2)^{1/2}|\widehat{E_1^k}(\tau,x)|^2dxd\tau\\&+\int_{\mathbb{R}}\int_{-\infty}^0\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})|\widehat{\partial_x E_1^k}(\tau,x)|^2dxd\tau\\&+\frac12\int_{\mathbb{R}}|\partial_x E_1^k(0,.)-\sqrt{-i\partial_t-V(0)-i\eta}E_1^k(0,.)|^2dt\\&\le\frac12\int_{\mathbb{R}}|\partial_x E_1^k(0,.)+\sqrt{-i\partial_t-V(0)-i\eta}E_1^k(0,.)|^2dt.\end{aligned}\tag{5.12}$$

Introducing the boundary operators $\mathcal{B}^+=\partial_x+\sqrt{-i\partial_t-V(0)-i\eta}$, and $\mathcal{B}^-=\partial_x-\sqrt{-i\partial_t-V(0)-i\eta}$ and the energy

$$\begin{aligned}J_1(w)=&\int_{\mathbb{R}}\int_{-\infty}^0\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})(\eta^2+(\tau-V(x))^2)^{1/2}|\widehat{w}(\tau,x)|^2dxd\tau\\&+\int_{\mathbb{R}}\int_{-\infty}^0\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})|\widehat{\partial_x w}(\tau,x)|^2dxd\tau\end{aligned}\tag{5.13}$$

we can rewrite (5.12) as:

$$J_1(E_1^k)+\frac12\int_{\mathbb{R}}|\mathcal{B}^-E_1^k|^2dt\le\frac12\int_{\mathbb{R}}|\mathcal{B}^+E_1^k|^2dt.\tag{5.14}$$

Similarly, we obtain for E_2^k

$$J_2(E_2^k)+\frac12\int_{\mathbb{R}}|\mathcal{B}^+E_2^k|^2dt\le\frac12\int_{\mathbb{R}}|\mathcal{B}^-E_2^k|^2dt\tag{5.15}$$

where the energy J_2 is defined by

$$\begin{aligned}J_2(w)=&\int_{\mathbb{R}}\int_0^{+\infty}\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})(\eta^2+(\tau-V(x))^2)^{1/2}|\widehat{w}(\tau,x)|^2dxd\tau\\&+\int_{\mathbb{R}}\int_0^{+\infty}\mathcal{R}e\,(\sqrt{\tau-V(x)-i\eta})|\widehat{\partial_x w}(\tau,x)|^2dxd\tau.\end{aligned}\tag{5.16}$$

Now note that the transmission conditions in (5.5) can be expressed with the operators $\mathcal{B}^{\pm}$ as

$$\mathcal{B}^- E_1^k(0,\cdot) = \mathcal{B}^- E_2^{k-1}(0,\cdot), \quad \mathcal{B}^+ E_2^k(0,\cdot) = \mathcal{B}^+ E_1^{k-1}(0,\cdot).$$

Replacing the corresponding terms in the equations (5.14) and (5.15), and adding, we find

$$J_1(E_1^k) + J_2(E_2^k) + \frac{1}{2}\int_{\mathbb{R}} (|\mathcal{B}^- E_1^k|^2 + |\mathcal{B}^+ E_2^k|^2) dt \leq \frac{1}{2}\int_{\mathbb{R}} (|\mathcal{B}^- E_1^{k-1}|^2 + |\mathcal{B}^+ E_2^{k-1}|^2) dt. \tag{5.17}$$

Summing (5.17) in k, we get a telescopic sum on the interfaces and therefore

$$\begin{aligned} &\sum_{k=1}^{K} (J_1(E_1^k) + J_2(E_2^k)) \\ &\qquad + \frac{1}{2}\int_{\mathbb{R}} (|\mathcal{B}^- E_1^K|^2 + |\mathcal{B}^+ E_2^K|^2) dt \leq \frac{1}{2}\int_{\mathbb{R}} (|\mathcal{B}^- E_1^0|^2 + |\mathcal{B}^+ E_2^0|^2) dt. \end{aligned} \tag{5.18}$$

The sum of the energies over all the iterates remains bounded. Hence the energy $J_1(E_1^k) + J_2(E_2^k)$ needs to go to zero.

Finally, using (5.10) and the definitions (5.13) and (5.16) of J_1 and J_2, we see that

$$J_1(w) \geq \|w\|^2_{H^{1/4}(0,T,L^2(\Omega_1))} + \|\partial_x w\|^2_{H^{-1/4}(0,T,L^2(\Omega_1))} \tag{5.19}$$

and

$$J_2(w) \geq \|w\|^2_{H^{1/4}(0,T,L^2(\Omega_2))} + \|\partial_x w\|^2_{H^{-1/4}(0,T,L^2(\Omega_2))}. \tag{5.20}$$

Therefore, the algorithm (5.1) converges in

$$(H^{1/4}(0,T,L^2(\Omega_1)) \cap H^{-1/4}(0,T,H^1(\Omega_1))) \times (H^{1/4}(0,T,L^2(\Omega_2)) \cap H^{-1/4}(0,T,H^1(\Omega_2))).$$

■

6 The Algorithm with Robin Transmission Conditions

A simple alternative to the previous approach is to use Robin transmission conditions, *i.e.* to replace the optimal operators $\mathcal{S}_j$ by $\mathcal{S}_1 = -\mathcal{S}_2 = -ipI$ where p is a real number.

$$\begin{cases} \mathcal{L}u_1^k = f \text{ in } \Omega_1 \times (0,T), \\ u_1^k(\cdot,0) = u_0 \text{ in } \Omega_1, \\ (\partial_x - ip)u_1^k(L,\cdot) = (\partial_x - ip)u_2^{k-1}(L,\cdot) \text{ in } (0,T), \end{cases} \begin{cases} \mathcal{L}u_2^k = f \text{ in } \Omega_2 \times (0,T), \\ u_2^k(\cdot,0) = u_0 \text{ in } \Omega_2, \\ (\partial_x + ip)u_2^k(0,\cdot) = (\partial_x + ip)u_1^{k-1}(0,\cdot) \text{ in } (0,T). \end{cases} \tag{6.1}$$

Remark 6.1 *This choice of transmission operators corresponds to the lower order rational approximation of the optimal operator introduced in [11].*

In this case the convergence factor ρ is equal to

$$\rho(\tau,p,L) = \left(\frac{ip + (\tau - V)^{1/2}}{ip - (\tau - V)^{1/2}}\right)^2 e^{-2(\tau-V)^{1/2}L}, \tag{6.2}$$

and thus we have $|\rho(\tau,p,L)| = e^{-2\sqrt{\tau-V}L}$ if $\tau \geq V$, and $|\rho(\tau,p,L)| = \left|\frac{p-\sqrt{-\tau+V}}{p+\sqrt{-\tau+V}}\right|^2$ if $\tau < V$. Therefore, in order for the algorithm to converge, we shall need that $p > 0$.

The algorithm is initialized by using only boundary data, therefore we define formally

$$g_L := (\partial_x - ip)u_2^0(L,\cdot), \quad g_0 := (\partial_x + ip)u_1^0(0,\cdot).$$

6.1 Well Posedness of the Algorithm

Without loss of generality, we only study the well posedness of the subdomain problem on Ω_1,

$$\begin{cases} \mathcal{L}v = f \text{ in } \Omega_1 \times (0,T), \\ v(\cdot,0) = u_0 \text{ in } \Omega_1, \\ (\partial_x v - ipv)(L,\cdot) = g \text{ in } (0,T). \end{cases} \tag{6.3}$$

The following proposition gives existence, uniqueness and regularity of the solution.

Proposition 6.2 *Let the real potential V be in $L^\infty(\Omega_1)$. Suppose f is in $H^1(0,T;L^2(\Omega_1))$, u_0 in $H^2(\Omega_1)$, g in $H^1(0,T)$, with the compatibility conditions*

$$\partial_x u_0(L) - ipu_0(L) = g(0). \tag{6.4}$$

Then, for $p > 0$, problem (6.3) has a unique solution v in $H^{2,1}(\Omega_1 \times (0,T))$. Furthermore, suppose V is constant, f is in $H^2((0,T)\times\Omega_1)$, u_0 in $H^4(\Omega_1)$. Then $v(0,\cdot)$ and $\partial_x v(0,\cdot)$ are in $H^1(0,T)$, and the following compatibility relation is satisfied:

$$\lim_{t\to 0_+} (\partial_x v(0,t) + ipv(0,t)) = \partial_x u_0(0) + ipu_0(0). \tag{6.5}$$

Proof (i) First *a priori* estimates. Multiplying equation (6.3) by $\bar{v}$, integrating by parts in space, using the boundary condition and taking the imaginary part, we obtain

$$\frac{1}{2}\frac{d}{dt}\|v(\cdot,t)\|^2 + p|v(L,t)|^2 = \mathcal{I}m\left((f(\cdot,t),v(\cdot,t)) - g(t)\bar{v}(L,t)\right), \tag{6.6}$$

where we have used the fact that the potential V is real. By the Cauchy-Schwarz inequality, and applying (2.5) to both terms of the right-hand side, we get after an integration in time

$$\begin{aligned} \|v(\cdot,t)\|^2 + p\int_0^t |v(L,s)|^2\,ds \leq\ & \|u_0\|^2 + \int_0^t \|f(\cdot,s)\|^2\,ds + \frac{1}{p}\int_0^t |g(s)|^2\,ds \\ & + \int_0^t \|v(\cdot,s)\|^2\,ds. \end{aligned} \tag{6.7}$$

Applying the Gronwall Lemma gives the first bounds for v:

$$\|v\|^2_{L^\infty(0,T;L^2(\Omega_1))} + p\|v(L,\cdot)\|^2_{L^2(0,T)} \leq e^T(\|u_0\|^2 + \|f\|^2_{L^2(0,T;L^2(\Omega_1))} + \frac{1}{p}\|g\|^2_{L^2(0,T)}). \tag{6.8}$$

We apply (6.8) to $\partial_t v$, with the initial condition $\partial_t v(\cdot,0) = -i(f(\cdot,0) - \partial_{xx}u_0 - Vu_0) \in L^2(\Omega_1)$. By the regularity assumptions on the data, and the Trace Theorem in time for f, we obtain

$$\begin{aligned} \|\partial_t v\|^2_{L^\infty(0,T;L^2(\Omega_1))} + \|\partial_t v(L,\cdot)\|^2_{L^2(0,T)} \leq Ce^T(&\|u_0\|^2_{H^2(\Omega_1)} + \|V\|^2_{L^\infty(\Omega_1)}\|u_0\|^2_{L^2(\Omega_1)} \\ &+ \|f\|^2_{H^1(0,T;L^2(\Omega_1))} + \frac{1}{p}\|g\|^2_{H^1(0,T)}). \end{aligned} \tag{6.9}$$

(ii) Second *a priori* estimates. We now multiply equation (6.3) by $\partial_t\bar{v}$, integrate by parts in space, using the boundary condition, and take the real part. We obtain

$$-\frac{d}{dt}\|\partial_x v\|^2 + 2p\,\mathcal{R}e\, iv(L,\cdot)\partial_t\bar{v}(L,\cdot) = -2\mathcal{R}e\,(g\partial_t\bar{v}(L,\cdot)) + 2\mathcal{R}e\,(Vv(\cdot,t),\partial_t\bar{v}(\cdot,t)) + 2\mathcal{R}e\,(f(\cdot,t),\partial_t\bar{v}(\cdot,t)),$$

which implies

$$\begin{aligned} \|\partial_x v(\cdot,t)\|^2 \leq\ & p\|v(L,\cdot)\|^2_{L^2(0,T)} + (p+1)\|\partial_t v(L,\cdot)\|^2_{L^2(0,T)} + 2\|\partial_t v\|^2_{L^2((0,T)\times\Omega_1)} \\ & + \|V\|^2_{L^\infty(\Omega_1)}\|v\|^2_{L^2((0,T)\times\Omega_1)} + \|f\|^2_{L^2((0,T)\times\Omega_1)} + \|g\|^2_{L^2(0,T)} + \|\partial_x u_0\|^2, \end{aligned}$$

and by (6.8), (6.9),

$$\|\partial_x v(\cdot,t)\|^2_{L^\infty(0,T;L^2(\Omega_1))} \leq Ce^T(\|u_0\|^2_{H^2(\Omega_1)} + \|V\|^2_{L^\infty(\Omega_1)}\|u_0\|^2_{L^2(\Omega_1)} + \|f\|^2_{H^1(0,T;L^2(\Omega_1))} + \|g\|^2_{H^1(0,T)}). \tag{6.10}$$

Finally, using the equation $\mathcal{L}v = f$ and (6.9), we have

$$\|\partial_{xx}v(\cdot,t)\|^2_{L^\infty(0,T;L^2(\Omega_1))} \le Ce^T(\|u_0\|^2_{H^2(\Omega_1)} + \|V\|^2_{L^\infty(\Omega_1)}\|u_0\|^2_{L^2(\Omega_1)} + \|f\|^2_{H^1(0,T;L^2(\Omega_1))} + \|g\|^2_{H^1(0,T)}). \tag{6.11}$$

By (6.8),(6.9),(6.10) and (6.11), we have a bound on v in $H^{2,1}(\Omega_1 \times (0,T))$, and on $v(L,\cdot)$ in $H^1(0,T)$. This is sufficient to obtain existence and uniqueness in these spaces by the Galerkin method. Furthermore, by the Trace Theorem in $H^{2,1}(\Omega_1 \times (0,T))$, we have $v(0,\cdot)$ in $H^{3/4}(0,T)$.

(*iii*) Third *a priori* estimates.
We now prove that $v(0,\cdot)$ is actually in $H^1(0,T)$. With the additional assumptions on the data, the solution u of (2.1), (2.2) is in $H^{4,2}(\Omega_1 \times (0,T))$ [6]. We use the same sketch as in Proposition 3.1: we introduce the auxiliary problem satisfied by $z = e^{-t}(v-u)$ in $\Omega_1 \times (0,T)$:

$$\begin{cases} i\partial_t z + iz + \partial_{xx}z + Vz = 0 \text{ in } \Omega_1 \times (0,T), \\ z(\cdot,0) = 0 \text{ in } \Omega_1, \\ \partial_x z(L,\cdot) = ipz(L,\cdot) + h \text{ in } (0,T), \end{cases} \tag{6.12}$$

with $h(t) = e^{-t}(g(t) - \partial_x u(L,t) + ipu(L,t))$. The boundary data h is in $H^1(0,T)$. Due to the compatibility conditions (6.4), we can extend h in $H^1(\mathbb{R})$ by H, vanishing for negative t, and we have through Fourier transform in time,

$$\hat{z}(x,\tau) = \frac{\widehat{H}(\tau)}{(\tau - V - i)^{1/2} - ip} e^{-(\tau-V-i)^{1/2}(L-x)}, \; x < L. \tag{6.13}$$

Since $\mathcal{I}m\,(\tau - V - i)^{1/2} \le 0$, we have $|\hat{z}(0,\tau)| \le \frac{1}{p}|\widehat{H}(\tau)|$, and

$$\|z(0,\cdot)\|_{H^1(0,T)} \le \frac{1}{p}\|h\|_{H^1(0,T)},$$

which proves that $v(0,\cdot)$ is in $H^1(0,T)$, and

$$\|v(0,\cdot)\|^2_{H^1(0,T)} \le Ce^T(\|u\|^2_{H^{4,2}(\Omega_1\times(0,T))} + \|g\|^2_{H^1(0,T)}). \tag{6.14}$$

To conclude the proof of the Proposition, we need to prove (6.5). Since u is in $H^{4,2}(\Omega_1 \times (0,T))$, it satisfies

$$\lim_{t\to 0_+} (\partial_x u(0,t) + ipu(0,t)) = \partial_x u_0(0) + ipu_0(0).$$

Therefore we only need to prove that

$$\lim_{t\to 0_+} (\partial_x z(0,t) + ipz(0,t)) = 0.$$

Since $h(0) = 0$, using the boundary condition, this amounts to proving that $\lim_{t\to 0_+} z(0,t) = 0$, which can be established as in Proposition 3.1.

■

The same result also holds on subdomain Ω_2, leading to an existence result for the algorithm:

Theorem 6.3 *Let V be a real constant. Let $p > 0$, and let g_L and g_0 be given in $H^1(0,T)$, with the compatibility conditions*

$$\partial_x u_0(L) - ipu_0(L) = g_L(0), \quad \partial_x u_0(0) + ipu_0(0) = g_0(0). \tag{6.15}$$

Then (6.1) define a sequence of iterates (u_1^k, u_2^k) in $H^{2,1}(\Omega_1 \times (0,T)) \times H^{2,1}(\Omega_2 \times (0,T))$, with $u_1^k(0,\cdot)$, $\partial_x u_1^k(0,\cdot)$, $u_2^k(L,\cdot)$ and $\partial_x u_2^k(L,\cdot)$ in $H^1(0,T)$. Furthermore, at each step k, the following compatibility relations are fulfilled:

$$\begin{aligned} &\lim_{t\to 0_+} (\partial_x u_1^k(0,t) + ipu_1^k(0,t)) = \partial_x u_0(0) + ipu_0(0), \\ &\lim_{t\to 0_+} (\partial_x u_2^k(L,t) - ipu_2^k(L,t)) = \partial_x u_0(L) - ipu_0(L). \end{aligned} \tag{6.16}$$

Proof The proof is done by induction using Proposition 6.2. ■

6.2 Convergence of the Overlapping Algorithm

Let h_L and h_0 be given in $H^1(0,T)$. Let (e_1, e_2) be the solution in $H^{2,1}(\Omega_1 \times (0,T)) \times H^{2,1}(\Omega_2 \times (0,T))$ of the problem

$$\begin{cases} \mathcal{L}e_1 = 0 \text{ in } \Omega_1 \times (0,T), \\ e_1(\cdot,0) = 0 \text{ in } \Omega_1, \\ (\partial_x - ip)e_1(L,\cdot) = h_L \text{ in } (0,T), \end{cases} \quad \begin{cases} \mathcal{L}e_2 = 0 \text{ in } \Omega_2 \times (0,T), \\ e_2(\cdot,0) = 0 \text{ in } \Omega_2, \\ (\partial_x + ip)e_2(0,\cdot) = h_0 \text{ in } (0,T). \end{cases} \tag{6.17}$$

Lemma 6.4 *Let V be a real constant. For $L > 0$ and $p > 0$, the map $\mathcal{G}_0$ associated with (6.17),*

$$\mathcal{G}_0 : (e^{-t}h_L, e^{-t}h_0) \mapsto (e^{-t}(\partial_x e_2 - ipe_2)(L,\cdot), e^{-t}(\partial_x e_1 + ipe_1)(0,\cdot)), \tag{6.18}$$

is a contraction of $({}_0H^1(0,T))^2$. The local convergence factor is defined as

$$\theta_0(\tau, L) = -\frac{(\tau - V - i)^{1/2} + ip}{(\tau - V - i)^{1/2} - ip}\, \theta_D(\tau, L). \tag{6.19}$$

Moreover, if there is $\tau_{max} > 0$ such that $\widehat{e^{-t}h_L}$ and $\widehat{e^{-t}h_0}$ vanish outside $[-\tau_{max}, +\infty)$, then $\mathcal{G}_0$ is a strict contraction:

$$\|\mathcal{G}_0(e^{-t}h_L, e^{-t}h_0)\|_{(H^1(0,T))^2} \leq \Theta_0(\tau_{max}, L)\|(e^{-t}h_L, e^{-t}h_0)\|_{(H^1(0,T))^2} \tag{6.20}$$

with $\Theta_0(\tau_{max}, L) = sup_{\tau\in[-\tau_{max},+\infty)}|\theta_0(\tau, L)| < 1$.

Proof The proof is analogous to the proof of Lemma 3.4 using Fourier analysis. We can multiply h_L and h_0 in ${}_0H^1(0,T)$ by e^{-t}, extend the result by H_L and H_0 in $H^1(\mathbb{R})$, vanishing on $(-\infty, 0)$, extend (6.17) in time on $\mathbb{R}$, define $E_j = e_j e^{-t}$, and Fourier transform the resulting equation in time. We obtain:

$$\hat{E}_1(x,\tau) = \frac{\widehat{H}_L(\tau)}{(\tau - V - i)^{1/2} - ip} e^{-(\tau-V-i)^{1/2}(L-x)}, \quad \hat{E}_2(x,\tau) = \frac{\widehat{H}_0(\tau)}{-(\tau - V - i)^{1/2} + ip} e^{-(\tau-V-i)^{1/2}x},$$

which gives $\mathcal{F}(\mathcal{G}_0(e^{-t}h_L, e^{-t}h_0))(\tau) = \theta_0(\tau, L)(\mathcal{F}(e^{-t}h_0, e^{-t}h_L)(\tau))$, and

$$|\mathcal{F}(\mathcal{G}_0(e^{-t}h_L, e^{-t}h_0))(\tau)| \leq \sup_{\tau\in[-\tau_{max},+\infty)} |\theta_0(\tau, L)||(\mathcal{F}(e^{-t}h_0)(\tau), \mathcal{F}(e^{-t}h_L)(\tau))|.$$

Since $p > 0$, we have $\sup_{\tau\in[-\tau_{max},+\infty)} |\theta_0(\tau, L)| \leq \Theta_D(\tau_{max}, L)$, and thus

$$\|\mathcal{G}_0(h_L, h_0)\|_{(H^1(0,T))^2} \leq \Theta_D(\tau_{max}, L)\|(h_L, h_0)\|_{(H^1(0,T))^2}.$$

Since $\Theta_D(\tau_{max}, L) < 1$, the result follows. ■

From the proof of this Lemma, we can see that the contraction of the overlapping Schwarz waveform relaxation map with Robin transmission conditions, $\mathcal{G}_0$ given in (6.18), is at least as good as the contraction of the classical map with Dirichlet transmission conditions, $\mathcal{G}_D$ given in (3.12), whatever choice we make for the parameter $p > 0$ in the Robin transmission conditions. We use now the contraction property from Lemma 6.4 to prove convergence of the new algorithm.

Theorem 6.5 *Let V be a real constant. Let an initial guess (g_0, g_L) in $(H^1(0,T))^2$ such that the compatibility conditions (6.15) are fulfilled. Suppose $h_0 = g_0 - \partial_x u(0,\cdot) - ipu(0,\cdot)$ and $h_L = g_L - \partial_x u(L,\cdot) + ipu(L,\cdot)$ are such that $\widehat{e^{-t}h_L}$ and $\widehat{e^{-t}h_0}$ vanish outside $[-\tau_{max}, +\infty)$. For $p > 0$, the solution (u_1^k, u_2^k) of algorithm (6.1) converges in $L^2(\Omega_1 \times (0,T)) \times L^2(\Omega_2 \times (0,T))$ to the solution u of (2.1).*

Proof We define the errors $e_j^k = u_j^k - u$, $j = 1, 2$, solution of the homogeneous algorithm, and introduce the interface functions $h_L^k = (\partial_x e_2^k - ipe_2^k)(L,\cdot)$ and $h_0^k = (\partial_x e_1^k + ipe_1^k)(0,\cdot)$. Using the map $\mathcal{G}_0$, we obtain by induction

$$(e^{-t}h_L^k, e^{-t}h_0^k) = \mathcal{G}_0^k(e^{-t}h_L^0, e^{-t}h_0^0), \text{ for } k \text{ even, } (e^{-t}h_L^k, e^{-t}h_0^k) = \mathcal{G}_0^k(e^{-t}h_0^0, e^{-t}h_L^0) \text{ for } k \text{ odd.}$$

By Lemma 6.4, we have

$$\|(e^{-t}h_L^k, e^{-t}h_0^k)\|_{(H^1(0,T))^2} \leq (\Theta_0(\tau_{max}, L))^k\|(e^{-t}h_L^0, e^{-t}h_0^0)\|_{(H^1(0,T))^2}.$$

In the same way as in (3.6), we obtain with obvious notations the exact formula

$$\widehat{e^{-t}e_1^k}(x,\tau) = \frac{\widehat{H_1^{k-1}}(\tau)}{(\tau - V - i)^{1/2} - ip} e^{-(\tau-V-i)^{1/2}(L-x)},\ x < L. \tag{6.21}$$

Since $|(\tau - V - i)^{1/2} - ip| \geq p$, we have as in (3.9),

$$\|e^{-t}e_1^k\|_{L^2(0,T,L^2(\Omega_1))} \leq \frac{1}{p} \left\|e^{-t}h_L^{k-1}\right\|_{H^{1/4}(0,T)} \leq \frac{1}{p} \left\|e^{-t}h_L^{k-1}\right\|_{H^1(0,T)}. \tag{6.22}$$

An estimate of the form (6.22) also holds for e_2^k, and we finally have like in (3.20),

$$\|e_j^k\|_{L^2(\Omega_j \times (0,T))} \leq e^T \Theta_0(\tau_{max}, L)^{k-1} \|(h_L^0, h_0^0)\|_{(H^1(0,T))^2}, \tag{6.23}$$

which completes the proof. ■

6.3 Convergence for the Non-Overlapping Algorithm

We now assume that there is no overlap, *i.e.* $L = 0$. We first analyze the convergence of the algorithm in the appropriate Sobolev spaces. The convergence analysis for the non-overlapping case is based on energy estimates and follows an idea from [7], which has widely been used since (see [3], [8] for steady problems, [5] for evolution equations).

Theorem 6.6 *Without overlap, $L = 0$, the Schwarz waveform relaxation algorithm (6.1) converges for $p > 0$ in $L^\infty(0,T;L^2(\Omega_1)) \times L^\infty(0,T;L^2(\Omega_2))$ to the solution u of (2.1), (2.2) for any initial guess (g_0, g_L) in $(H^1(0,T))^2$ and any real potential V in $L^\infty(\mathbb{R})$.*

Proof We use the energy estimate (6.6) in Ω_1 for the error e_1^k, and the corresponding energy estimate in Ω_2 for the error e_2^k,

$$\frac{1}{2}\frac{d}{dt}\|e_1^k\|^2 + \mathcal{I}m\,(\partial_x e_1^k(0)\,\overline{e_1^k(0)}) = 0, \tag{6.24}$$

$$\frac{1}{2}\frac{d}{dt}\|e_2^k\|^2 - \mathcal{I}m\,(\partial_x e_2^k(0)\,\overline{e_2^k(0)}) = 0. \tag{6.25}$$

Introducing the boundary operators $\mathcal{B}^+ = \partial_x + ip$, $\mathcal{B}^- = \partial_x - ip$, and rewriting the terms on the interface in the form

$$\mathcal{I}m\,(\partial_x e(0,\cdot)\,\overline{e(0,\cdot)}) = \frac{1}{4p}(|\mathcal{B}^+e(0,\cdot)|^2 - |\mathcal{B}^-e(0,\cdot)|^2),$$

we obtain the new energy estimates

$$\frac{1}{2}\frac{d}{dt}\|e_1^k\|^2 + \frac{1}{4p}|\mathcal{B}^+e_1^k(0,\cdot)|^2 = \frac{1}{4p}|\mathcal{B}^-e_1^k(0,\cdot)|^2, \tag{6.26}$$

$$\frac{1}{2}\frac{d}{dt}\|e_2^k\|^2 + \frac{1}{4p}|\mathcal{B}^-e_2^k(0,\cdot)|^2 = \frac{1}{4p}|\mathcal{B}^+e_2^k(0,\cdot)|^2. \tag{6.27}$$

Now note that the transmission conditions can be expressed with the operators $\mathcal{B}^\pm$ as

$$\mathcal{B}^-e_1^k(0,\cdot) = \mathcal{B}^-e_2^{k-1}(0,\cdot), \quad \mathcal{B}^+e_2^k(0,\cdot) = \mathcal{B}^+e_1^{k-1}(0,\cdot).$$

Replacing the corresponding terms in the two equations (6.26) and (6.27), we find

$$\frac{d}{dt}\|e_1^k\|^2 + \frac{1}{2p}|\mathcal{B}^+e_1^k(0,\cdot)|^2 = \frac{1}{2p}|\mathcal{B}^-e_2^{k-1}(0,\cdot)|^2, \tag{6.28}$$

$$\frac{d}{dt}\|e_2^k\|^2 + \frac{1}{2p}|\mathcal{B}^-e_2^k(0,\cdot)|^2 = \frac{1}{2p}|\mathcal{B}^+e_1^{k-1}(0,\cdot)|^2. \tag{6.29}$$

Adding these two equations and summing in k, we get a telescopic sum on the interfaces and therefore

$$\sum_{k=1}^{K} \frac{d}{dt}(\|e_1^k\|^2 + \|e_2^k\|^2) + \frac{1}{2p}(|\mathcal{B}^+e_1^K|^2 + |\mathcal{B}^-e_2^K|^2)(0,\cdot) = \frac{1}{2p}(|\mathcal{B}^+e_1^0|^2 + |\mathcal{B}^-e_2^0|^2)(0,\cdot). \tag{6.30}$$

We can now integrate in time, and since the initial values of the error vanish, the sum of the energies over all the iterates remains bounded. Hence the energy in the iterates needs to go to zero and the algorithm converges. ■

6.4 Optimization of the Algorithm with Overlap

We suppose here the potential to be constant. According to (6.2), the convergence factor associated to Robin transmission conditions is

$$\rho(\tau,p,L) = \Big(\frac{ip+(\tau-V)^{1/2}}{ip-(\tau-V)^{1/2}}\Big)^2 e^{-2\tau^{1/2}L}, \tag{6.31}$$

In practical computations, only a bounded range of frequencies are present: $|\tau| \in [\tau_{min}, \tau_{max}]$. For a discretization with time-step Δt, we have $\tau_{max} = \pi/\Delta t$, $\tau_{min} = \pi/T$. We define $D = (-\tau_{max}, -\tau_{min}) \cup (\tau_{min}, \tau_{max})$, and for a given potential V, the evanescent region $E_V = \{\tau \in D, \tau > V\}$, and the propagating region $P_V = \{\tau \in D, \tau < V\}$. The modulus $R(\tau,p,L)$ of the convergence factor is given by:

$$R(\tau,p,L) = \left\{ \begin{array}{ll} e^{-2\sqrt{\tau-V}L} & \text{if } \tau > V, \text{ evanescent region } E_V \\ \left(\dfrac{p-\sqrt{V-\tau}}{p+\sqrt{V-\tau}}\right)^2 & \text{if } \tau < V, \text{ propagating region } P_V. \end{array} \right. \tag{6.32}$$

In order to accelerate the convergence of the algorithm, we want to find a real positive number p which minimizes R over D. Since the behavior of R in E_V does not depend on p, we can only minimize the convergence factor in the propagating region. The following min max problem is the key of the minimization in P_V. We introduce the function

$$f(s,p) = \left(\frac{p-s}{p+s}\right)^2, \tag{6.33}$$

and the best approximation problem: find $p^* > 0$ such as to realize

$$\inf_{p>0} \sup_{s\in(s_{min},s_{max})} f(s,p). \tag{6.34}$$

Problem (6.34) is quite simple and can be treated at hand.

Lemma 6.7 *The best approximation problem (6.34) has a unique solution p^*, defined by $f(s_{min},p^*) = f(s_{max},p^*)$, and given by*

$$p^* = (s_{min}s_{max})^{1/2}, s^* = s_{min}, f^* = f(s^*,p^*) = \left(\frac{\sqrt{s_{max}}-\sqrt{s_{min}}}{\sqrt{s_{max}}+\sqrt{s_{min}}}\right)^2.$$

Proof It is easy to see that for any positive p,

$$\sup_{s\in(s_{min},s_{max})} \left(\frac{p-s}{p+s}\right)^2 = \left\{ \begin{array}{ll} \left(\dfrac{s_{max}-p}{s_{max}+p}\right)^2 & \text{if } p \le \sqrt{s_{max}s_{min}}, \\ \left(\dfrac{p-s_{min}}{p+s_{min}}\right)^2 & \text{if } p \ge \sqrt{s_{max}s_{min}}. \end{array} \right.$$

The function $p \mapsto \sup_{s\in[s_{min},s_{max}]}\left(\dfrac{p-s}{p+s}\right)^2$ is now decreasing on $(0, \sqrt{s_{max}s_{min}})$ and increasing on $(\sqrt{s_{max}s_{min}}, +\infty)$. It has a unique minimum, attained for $p^* = \sqrt{s_{max}s_{min}}$. ■

We are able now to study the minimization of the convergence rate over the propagating region, and to calculate the optimal value. In the sequel $\lfloor s \rfloor$ is $floor(s)$, the integer part of the real number s, and $\lceil s \rceil$ is $ceil(s) = floor(s) + 1$.

Case 1, $V < -\tau_{max}$: $P_V = \emptyset$, $E_V = D$.

$$\forall p > 0, \max_{\tau\in D} R = e^{-2L\sqrt{-\tau_{max}-V}}.$$

Case 2, $-\tau_{max} < V < -\tau_{min}$: $P_V = (-\tau_{max}, V)$, $E_V = (V, -\tau_{min}) \cup (\tau_{min}, \tau_{max})$.

In this case, $\max_{\tau\in D} R = 1$. However, we can make a more precise analysis. In the discrete case, τ takes only discrete values $\tau_k = k\pi/T$, for $1 \le k \le K = \frac{T}{\Delta t}$. If $-V$ is none of the τ_k, we can consider values of τ in $(-\tau_{max}, -\tau_-) \cup (-\tau_+, -\tau_{min}) \cup (\tau_{min}, \tau_{max})$ with $\tau_- = \lceil \frac{-V}{\tau_{min}} \rceil \tau_{min}$, $\tau_+ = \lfloor \frac{-V}{\tau_{min}} \rfloor \tau_{min}$. We now have $P_V = (-\tau_{max}, -\tau_-)$, and by Lemma 6.7, $\max_{\tau\in P_V} R$ is minimal when $p = p^* = ((V+\tau_{max})(V+\tau_-))^{1/4}$, and is equal to $R(-\tau_{max}, p^*, L) = R(-\tau_-, p^*, L)$.

$$p^* = ((V+\tau_{max})(V+\tau_-))^{1/4}, \ \max_{\tau\in D} R(\tau, p^*, L) = \max\left(\frac{(V+\tau_{max})^{1/4} - (V+\tau_-)^{1/4}}{(V+\tau_{max})^{1/4} + (V+\tau_-)^{1/4}}, e^{-2L\sqrt{\tau_{min}-V}}\right).$$

Case 3, $-\tau_{min} < V < \tau_{min}$: $P_V = (-\tau_{max}, -\tau_{min})$, $E_V = (\tau_{min}, \tau_{max})$.

By Lemma 6.7, the norm of R in P_V is minimal for $p^* = ((V+\tau_{min})(V+\tau_{max}))^{1/4}$. The corresponding convergence factor is $R(-\tau_{max}, p^*, L)$. On the other hand, $max_{E_V} R = e^{-2L\sqrt{\tau_{min}-V}}$.

$$p^* = ((V+\tau_{min})(V+\tau_{max}))^{1/4}, \ \max_{\tau\in D} R(\tau, p^*, L) = \max\left(\frac{(V+\tau_{max})^{1/4} - (V+\tau_{min})^{1/4}}{(V+\tau_{max})^{1/4} + (V+\tau_{min})^{1/4}}, e^{-2L\sqrt{\tau_{min}-V}}\right).$$

Note that this case includes the free Schrödinger equation, *i.e.* the case $V = 0$.

Case 4, $\tau_{min} < V < \tau_{max}$: $P_V = (-\tau_{max}, -\tau_{min}) \cup (\tau_{min}, V)$, $E_V = (V, \tau_{max})$.

Again $\max_{\tau\in D} R = 1$, and we introduce the frequencies , $\tau_- = \lfloor \frac{V}{\tau_{min}} \rfloor \tau_{min}$, $\tau_+ = \lceil \frac{V}{\tau_{min}} \rceil \tau_{min}$. We now have $P_V = (-\tau_{max}, -\tau_{min}) \cup (\tau_{min}, \tau_-)$, $E_V = (\tau_+, \tau_{max})$, and

$$\max_{P_V} R = \max\bigl(f(-\tau_{max} - V, p), f(-\tau_{min} - V, p), f(\tau_{min} - V, p), f(\tau_- - V, p)\bigr)$$

As a function of p, it is first equal to $f(-\tau_{max} - V, p)$, then to $f(\tau_- - V, p)$. It is minimal when these quantities are equal , *i.e.* when $p* = ((V - \tau_-)(V + \tau_{max}))^{1/4}$. The corresponding convergence factor is $R(-\tau_-, p^*, L)$.

$$p^* = ((V-\tau_-)(V+\tau_{max}))^{1/4}, \ \max_{\tau\in D} R(\tau, p^*, L) = \max\left(\frac{(V-\tau_-)^{1/4} - (V+\tau_{max})^{1/4}}{(V-\tau_-)^{1/4} + (V+\tau_{max})^{1/4}}, e^{-2L\sqrt{\tau_+-V}}\right).$$

Case 5, $V > \tau_{max}$: $P_V = D$, $E_V = \emptyset$. By Lemma 6.7, the minimum value is attained for $p^* = (V^2 - \tau_{max}^2)^{1/4}$, and $R^* = R(\tau_{max}, p^*, V)$.

$$p^* = (V^2 - \tau_{max}^2)^{1/4}, \ \max_{\tau\in D} R(\tau, p^*, L) = \max\bigl(\frac{(V+\tau_{max})^{1/4} - (V-\tau_{max})^{1/4}}{(V+\tau_{max})^{1/4} + (V-\tau_{max})^{1/4}}, e^{-2L\sqrt{\tau_+-V}}\bigr).$$

7 Construction of the Discrete Algorithms

7.1 Discretization of the equation

We first discretize (2.1). Δx and Δt are the discretization parameters in space and time respectively, the discrete points in space are denoted by $x_j = j\Delta x$, and in time $t^n = n\Delta t$, with $\Delta t = T/N$. The discrete difference operators are defined by

$$\begin{aligned} D_x^+ U(j,n) &= \frac{U(j+1,n) - U(j,n)}{\Delta x}, \quad D_x^- U(j,n) = \frac{U(j,n) - U(j-1,n)}{\Delta x}, \\ D_t^+ U(j,n) &= \frac{U(j,n+1) - U(j,n)}{\Delta t}, \qquad F(n+\frac{1}{2}) = \frac{1}{2}(F(n) + F(n+1)). \end{aligned} \tag{7.1}$$

We shall use the Crank Nicolson scheme

$$LU(j,n) := iD_t^+ U(j,n) + D_x^+ D_x^- U(j, n+\tfrac{1}{2}) + V(j)\, U(j, n+\tfrac{1}{2}) = F(j, n+\tfrac{1}{2}), \tag{7.2}$$

which is unconditionally stable, second order in time and space. The scheme is completed with the initial condition $U(j,0) = u_0(x_j)$.

7.2 Discretization of the classical Schwarz algorithm

We suppose that $L = \ell\Delta x$. The points in Ω_1 are numbered from $-\infty$ to ℓ, and the points in Ω_2 are numbered from 0 to $+\infty$. We denote the numerical approximation to $u_i^k(j\Delta x, n\Delta t)$ on Ω_i at iteration step k by $U_i^k(j,n)$. The discrete form of algorithm (3.1) is:

$$\begin{cases} iD_t^+ U_1^k(j,n) + D_x^+ D_x^- U_1^k(j,n+\frac{1}{2}) + V(j)\, U_1^k(j,n+\frac{1}{2}) = F(j,n+\frac{1}{2}) \text{ for } j \le \ell, 0 \le n \le N, \\ U_1^k(j,0) = U(j,0) \quad \text{for } j \le \ell, \\ U_1^k(\ell,n+\frac{1}{2}) = U_2^{k-1}(\ell,n+\frac{1}{2}) \text{ for } 0 \le n \le N, \end{cases}$$
$$\begin{cases} iD_t^+ U_2^k(j,n) + D_x^+ D_x^- U_2^k(j,n+\frac{1}{2}) + V(j)\, U_2^k(j,n+\frac{1}{2}) = F(j,n+\frac{1}{2}) \text{ for } j \ge 0, 0 \le n \le N, \\ U_2^k(j,0) = U(j,0) \text{ for } j \ge 0, \\ U_2^k(0,n+\frac{1}{2}) = U_1^{k-1}(0,n+\frac{1}{2}) \text{ for } 0 \le n \le N. \end{cases} \tag{7.3}$$

Remark 7.1 *Since the initial values are given for all discrete values, the transmission conditions in (7.3) are equivalent to* $U_1^k(\ell,n) = U_2^{k-1}(\ell,n)$ *and* $U_2^k(0,n) = U_1^{k-1}(0,n)$.

7.3 Discretization of the boundary value problem with Robin boundary condition

The Crank-Nicolson scheme can be obtained through a finite volumes procedure. This approach takes a better account of the Robin boundary condition, as was first noticed in [5], in relation with the Schwarz waveform relaxation for the wave equation. The function u is assumed to be a constant in $(x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}) \times (t_{n-\frac{1}{2}}, t_{n+\frac{1}{2}})$, with the notations $x_{j\pm\frac{1}{2}} = x_j \pm \Delta x/2$, $t_{n\pm\frac{1}{2}} = t_n \pm \Delta t/2$. Its derivative in time $\partial_t u$ is constant in $(x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}) \times (t_n, t_{n+1})$, equal to $D_t^+ U(j,n)$, and its derivative in space $\partial_x u$ is constant in $(x_j, x_{j+1}) \times (t_{n-\frac{1}{2}}, t_{n+\frac{1}{2}})$, equal to $D_x^+ U(j,n)$. The control volume around a grid point (x_j, t_n) is $D = (x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}) \times (t_n, t_{n+1})$. Integrating on D yields the Crank Nicolson scheme (7.2) in the interior. As for the boundary conditions, we start with the right boundary:

7.3.1 Construction of the discrete Robin boundary condition on the right boundary

We start with the continuous boundary condition

$$(\partial_x v - ipv)(L,\cdot) = g_r \text{ in } (0,T). \tag{7.4}$$

We first integrate the equation on the control volume $(x_{\ell-\frac{1}{2}}, x_\ell) \times (t_n, t_{n+1})$. For the time derivative we obtain

$$\int_{t_n}^{t_{n+1}} \int_{x_{\ell-\frac{1}{2}}}^{x_\ell} \partial_t u(x,t)\, dxdt \approx \frac{1}{2}\Delta x \Delta t D_t^+ U(\ell,n),$$

and for the second derivative in space

$$\int_{x_{\ell-\frac{1}{2}}}^{x_\ell} \int_{t_n}^{t_{n+1}} \partial_{xx} u(x,t)\, dxdt = \int_{t_n}^{t_{n+1}} \partial_x u(x_\ell,t)\, dt - \int_{t_n}^{t_{n+1}} \partial_x u(x_{l-\frac{1}{2}},t)\, dt.$$

The space derivative $\partial_x u(x_{l-\frac{1}{2}},t)$ is approximated on (t_n, t_{n+1}) by $D_x^- U(\ell, n+\frac{1}{2})$. Integrating all the terms leads to

$$\begin{aligned} & i\frac{1}{2}\Delta x \Delta t D_t^+ U(\ell,n) - \Delta t D_x^- U(\ell,n+\tfrac{1}{2}) + \int_{t_n}^{t_{n+1}} \partial_x u(x_\ell,t)\, dt \\ & + \frac{1}{2}\Delta x \Delta t V(\ell) U(\ell,n+\tfrac{1}{2}) = \frac{1}{2}\Delta x \Delta t F(\ell,n+\tfrac{1}{2}). \end{aligned} \tag{7.5}$$

In order to evaluate the time integral on the left, we integrate the boundary condition (7.4) on (t_n, t_{n+1}):

$$\int_{t_n}^{t_{n+1}} \partial_x u(x_\ell,t)\, dt - ip\Delta t U(\ell,n+\tfrac{1}{2}) \approx \int_{t_n}^{t_{n+1}} g_r(t)\, dt. \tag{7.6}$$

We define, for $n \geq 0$, $G_r(n) = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} g_r(t)\, dt$, and the boundary operator

$$B_r U(\ell, n) := D_x^- U(\ell, n+\tfrac{1}{2}) - ipU(\ell, n+\tfrac{1}{2}) - \frac{i}{2}\Delta x D_t^+ U(\ell, n) - \frac{\Delta x}{2} V(\ell) U(\ell, n+\tfrac{1}{2}), \tag{7.7}$$

and the discrete condition on the right boundary of Ω_1 is

$$B_r U(\ell, n) = \; G_r(n) - \frac{\Delta x}{2} \; F(\ell, n+\tfrac{1}{2}). \tag{7.8}$$

7.3.2 Construction of the discrete Robin boundary condition on the left boundary

The continuous boundary condition is

$$(\partial_x v + ipv)(L, \cdot) = g_l \text{ in } (0, T). \tag{7.9}$$

We first integrate the equation on the control volume $(x_0, x_{\frac{1}{2}}) \times (t_n, t_{n+1})$. For the time derivative we obtain

$$\int_{x_0}^{x_{\frac{1}{2}}} \int_{t_n}^{t_{n+1}} \partial_t u(x, t)\, dxdt \approx \frac{1}{2}\Delta x \Delta t D_t^+ U(0, n),$$

and for the second derivative in space

$$\int_{t_n}^{t_{n+1}} \int_{x_0}^{x_{\frac{1}{2}}} \partial_{xx} u(x, t)\, dxdt = \int_{t_n}^{t_{n+1}} \partial_x u(\tfrac{1}{2}, t)\, dt - \int_{t_n}^{t_{n+1}} \partial_x u(x_0, t)\, dt.$$

The space derivative $\partial_x u(x_{\frac{1}{2}}, t)$ is approximated by $D_x^+ U(0, n+\frac{1}{2})$, and we obtain

$$\begin{aligned} & i\frac{1}{2}\Delta x \Delta t D_t^+ U(0, n) + \Delta t D_x^+ U(0, n+\tfrac{1}{2}) - \int_{t_n}^{t_{n+1}} \partial_x u(x_0, t)\, dt \\ & + \frac{1}{2}\Delta x \Delta t V(0) U(0, n+\tfrac{1}{2}) = \frac{1}{2}\Delta x \Delta t F(0, n+\tfrac{1}{2}). \end{aligned} \tag{7.10}$$

To evaluate the integral on the left-hand side, we integrate the boundary condition (7.9) on (t_n, t_{n+1}):

$$\int_{t_n}^{t_{n+1}} \partial_x u(x_0, t)\, dt + ip\Delta t U(0, n+\tfrac{1}{2}) \approx \int_{t_n}^{t_{n+1}} g_l(t)\, dt. \tag{7.11}$$

We define, for $n \geq 0$, $G_l(n) = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} g_r(t)\, dt$, and the boundary operator for $0 \leq n \leq N$,

$$B_\ell U(0, n) := D_x^+ U(0, n+\tfrac{1}{2}) + ipU(0, n+\tfrac{1}{2}) + \frac{i}{2}\Delta x D_t^+ U(0, n) + \frac{\Delta x}{2} V(0) U(0, n+\tfrac{1}{2}). \tag{7.12}$$

The discrete condition on the right boundary of Ω_2 is

$$B_\ell U(0, n) = \frac{\Delta x}{2} \; F(0, n+\tfrac{1}{2}) + \; G_l(n). \tag{7.13}$$

We now describe the discrete algorithm.

7.4 The discrete Robin Schwarz relaxation algorithm

We first need in each subdomain to extract at step k the transmission conditions for the neighbor at step $k+1$.

7.4.1 Extraction of the transmission data in Ω_1

For u solution of the Schrödinger equation in Ω_1, and U an approximation with data G_r, we must now evaluate $\tilde{G}_l(n) = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} (\partial_x u + ipu)(0, t)\, dt$. We proceed as in (7.5), integrating the equation on the control domain $(x_{-\frac{1}{2}}, x_0) \times (t_n, t_{n+1})$, and obtain

$$\begin{aligned} & i\frac{1}{2}\Delta x \Delta t D_t^+ U(0, n) - \Delta t D_x^- U(0, n+\tfrac{1}{2}) + \int_{t_n}^{t_{n+1}} \partial_x u(x_0, t)\, dt \\ & + \frac{1}{2}\Delta x \Delta t V(0) U(0, n+\tfrac{1}{2}) = \frac{1}{2}\Delta x \Delta t F(0, n+\tfrac{1}{2}). \end{aligned}$$

Therefore we can evaluate $\tilde{G}_l$ by defining the extraction boundary operator $\tilde{B}_\ell U(n)$ by

$$\begin{aligned}
&\tilde{B}_\ell U(0,n) := D_x^- U(0,n+\tfrac{1}{2}) + ipU(0,n+\tfrac{1}{2}) - i\frac{\Delta x}{2} D_t^+ U(0,n) - \frac{\Delta x}{2} V(0)U(0,n+\tfrac{1}{2}),\\
&\tilde{G}_l U(n) = \tilde{B}_\ell U(0,n) + \frac{\Delta x}{2}\ F(0,n+\tfrac{1}{2}).
\end{aligned} \tag{7.14}$$

7.4.2 Extraction of the transmission data in Ω_2

For u solution of the Schrödinger equation in Ω_2, and U an approximation with data G_l, we must now evaluate $\tilde{G}_r(n) = \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} (\partial_x u - ipu)(\ell, t)\, dt$. We proceed as in (7.10), integrating the equation on the control domain $(x_\ell, x_{\ell+\frac{1}{2}}) \times (t_n, t_{n+1})$, and obtain

$$\begin{aligned}
&i\frac{1}{2}\Delta x \Delta t D_t^+ U(\ell,n) + \Delta t D_x^+ U(\ell, n+\tfrac{1}{2}) - \int_{t_n}^{t_{n+1}} \partial_x u(x_\ell, t)\, dt +\\
&\frac{1}{2}\Delta x \Delta t V(\ell) U(\ell, n+\tfrac{1}{2}) = \frac{1}{2}\Delta x \Delta t F(\ell, n+\tfrac{1}{2}).
\end{aligned}$$

Therefore we can evaluate $\tilde{G}_r$ by defining the extraction boundary operator $\tilde{B}_r U(n)$ by

$$\begin{aligned}
&\tilde{B}_r U(\ell,n) := D_x^+ U(\ell,n+\tfrac{1}{2}) - ipU(\ell,n+\tfrac{1}{2}) + i\frac{\Delta x}{2} D_t^+ U(\ell,n) + \frac{\Delta x}{2} V(\ell)U(\ell,n+\tfrac{1}{2}),\\
&\tilde{G}_r U(n) = \tilde{B}_r U(\ell,n) - \frac{\Delta x}{2}\ F(\ell,n+\tfrac{1}{2}).
\end{aligned} \tag{7.15}$$

Remark 7.2 (extraction of the Robin data without overlap) *In the case where $\ell = 0$, $\tilde{G}_l(n)$ is nothing else but $G_r(n) + 2ipU(0, n+\frac{1}{2})$, and $\tilde{G}_r(n) = G_l(n) - 2ipU(0, n+\frac{1}{2})$, which simplifies the procedure.*

7.4.3 The discrete algorithm

Let G_L^0 and G_0^0 be given. We define, for $k \geq 1$,

$$\begin{cases}
LU_1^k(j,n) = F(j,n+\tfrac{1}{2}) \ \text{ for } \ -\infty < j < \ell,\ 0 \leq n \leq N,\\
U_1^k(j,0) = u_0(x_j) \text{ for } \ -\infty < j \leq \ell,\\
B_r U_1^k(\ell,n) = \ G_L^{k-1}(n) - \dfrac{\Delta x}{2} F(\ell, n+\tfrac{1}{2}) \text{ for } 0 \leq n \leq N,
\end{cases} \tag{7.16}$$

$$\begin{cases}
LU_2^k(j,n) = F(j,n+\tfrac{1}{2}) \ \text{ for } 0 < j < +\infty,\ 0 \leq n \leq N,\\
U_2^k(j,0) = u_0(x_j) \text{ for } 0 \leq j < +\infty,\\
B_\ell U_2^k(0,n) = G_0^{k-1}(n) + \dfrac{\Delta x}{2}\ F(0,n+\tfrac{1}{2}) \ \text{ for } 0 \leq n \leq N,
\end{cases} \tag{7.17}$$

and compute

$$\begin{cases}
G_L^k(n) = \tilde{B}_r U_2^k(\ell,n) - \dfrac{\Delta x}{2}\ F(\ell,n+\tfrac{1}{2}) \text{ for } \ 0 \leq n \leq N,\\
G_0^k(n) = \tilde{B}_\ell U_1^k(0,n) + \dfrac{\Delta x}{2}\ F(0,n+\tfrac{1}{2}) \ \text{ for } \ 0 \leq n \leq N,
\end{cases} \tag{7.18}$$

where the discrete transmission operators B_j and $\tilde{B}_j$ are summarized below

$$\begin{aligned}
&B_r U_1(\ell,n) := D_x^- U_1(\ell,n+\tfrac{1}{2}) - ipU_1(\ell,n+\tfrac{1}{2}) - \frac{i}{2}\Delta x D_t^+ U_1(\ell,n) - \frac{\Delta x}{2} V(\ell)U_1(\ell,n+\tfrac{1}{2}),\\
&B_\ell U_2(0,n) := D_x^+ U_2(0,n+\tfrac{1}{2}) + ipU(0,n+\tfrac{1}{2})\frac{i}{2}\Delta x D_t^+ U_2(0,n) + \frac{\Delta x}{2} V(0)U(0,n+\tfrac{1}{2}),\\
&\tilde{B}_\ell U_1(0,n) := D_x^- U_1(0,n+\tfrac{1}{2}) + ipU_1(0,n+\tfrac{1}{2}) - i\frac{\Delta x}{2} D_t^+ U_1(0,n) - \frac{\Delta x}{2} V(0)U_1(0,n+\tfrac{1}{2}),\\
&\tilde{B}_r U_2(\ell,n) := D_x^+ U_2(\ell,n+\tfrac{1}{2}) - ipU_2(\ell,n+\tfrac{1}{2}) + i\frac{\Delta x}{2} D_t^+ U_2(\ell,n) + \frac{\Delta x}{2} V(\ell)U_2(\ell,n+\tfrac{1}{2}).
\end{aligned} \tag{7.19}$$

The previous formulas are useful for the practical implementation of the algorithm. In the forthcoming convergence analysis, we shall use the transmission conditions in the form

$$\begin{aligned} B_r U_1^k(\ell, n) &= \tilde{B}_r U_2^{k-1}(\ell, n) - \Delta x F(\ell, n + \tfrac{1}{2}), \\ B_\ell U_2^k(0, n) &= \tilde{B}_\ell U_1^{k-1}(0, n) + \Delta x F(0, n + \tfrac{1}{2}). \end{aligned} \tag{7.20}$$

7.5 The quasi optimal discrete algorithm

In [1] were designed discrete transparent boundary condition for the Crank Nicolson scheme, in the case of a constant potential outside the domain. They are given by

$$B_r^T U(\ell, n) := U(\ell - 1, n + 1) + U(\ell - 1, n) - \sum_{m=1}^{n+1} S_\ell(n - m + 1) U(\ell, m) = 0, \tag{7.21}$$

$$B_\ell^T U(0, n) := U(1, n + 1) + U(1, n) - \sum_{m=1}^{n+1} S_0(n - m + 1) U(0, m) = 0, \tag{7.22}$$

where the coefficients $S_j(m)$ are given by the table

$$\begin{aligned} &R = 2\frac{\Delta x^2}{\Delta t}, \ \sigma_j = -V(x_j)\Delta x^2, \ \alpha_j = \frac{i}{2}\, e^{i\phi_j/2}\big((R^2 + \sigma_j^2)(R^2 + (\sigma_j + 4)^2)\big)^{1/4}, \\ &\mu_j = \frac{(R^2 + 4\sigma_j + \sigma_j^2)}{\big((R^2 + \sigma_j^2)(R^2 + (\sigma_j + 4)^2)\big)^{1/2}}, \phi_j = \arctan\Big(2R\ \frac{\sigma_j + 2}{R^2 - 4\sigma_j - \sigma_j^2}\Big), \\ &S_j(0) = 1 - \frac{iR}{2} + \frac{\sigma_j}{2} - \alpha_j, \ S_j(1) = 1 + \frac{iR}{2} + \frac{\sigma_j}{2} + \alpha_j \mu_j e^{-i\phi_j}, \ S_j(2) = \frac{\alpha_j}{2} e^{-2i\phi_j}(\mu_j^2 - 1), \\ &S_j(m + 2) = \frac{2m - 1}{m + 1}\, \mu_j e^{-i\phi_j} S_j(m + 1) - \frac{m - 2}{m + 1}\, e^{-2i\phi_j} S_j(m), \ m \geq 1. \end{aligned} \tag{7.23}$$

Using these transparent boundary operators as transmission operator in the domain decomposition process, we write, for $k \geq 1$, and $1 \leq n \leq N$,

$$B_r^T U_1^k(\ell, n) = \ G_L^{k-1}(n), \quad B_\ell^T U_2^k(0, n) = G_0^{k-1}(n) \tag{7.24}$$

where, for $1 \leq n \leq N$,

$$\begin{aligned} G_L^k(n) &= 4U_2^k(\ell, n + \tfrac{1}{2}) - 2U_2^k(\ell + 1, n + \tfrac{1}{2}) - \sum_{m=1}^{n+1} S_\ell(n - m + 1) U_2^k(\ell, m) \\ &- 2i\frac{\Delta x^2}{\Delta t}(U_2^k(\ell, n + 1) - U_2^k(\ell, n)) - 2\Delta x^2 V(\ell) U_2^k(\ell, n + \tfrac{1}{2}) + 2\Delta x^2 F(\ell, n + \tfrac{1}{2}), \\ G_0^k(n) &= 4U_1^k(0, n + \tfrac{1}{2}) - 2U_1^k(-1, n + \tfrac{1}{2}) - \sum_{m=1}^{n+1} S_0(n - m + 1) U_1^k(0, m) \\ &- 2i\frac{\Delta x^2}{\Delta t}(U_1^k(0, n + 1) - U_1^k(0, n)) - 2\Delta x^2 V(0) U_1^k(0, n + \tfrac{1}{2}) + 2\Delta x^2 F(0, n + \tfrac{1}{2}). \end{aligned} \tag{7.25}$$

Here, we do not find G_0 and G_L through a finite volume procedure. Instead, we simply choose G_0 and G_L such that we obtain the Crank Nicolson scheme (7.2) when $U = U_1 = U_2$ (*i.e.* after the domain decomposition method has converged).

8 Convergence of the Discrete Algorithms

For the overlapping algorithms, the convergence will be obtained by a normal modes analysis, whereas energy estimates will prove the convergence in the non-overlapping case. We start by the study of the discrete Crank Nicolson scheme.

8.1 The Crank Nicolson scheme

In this section, V is a real constant. We introduce the normal mode analysis, as described in [10]. The discrete Laplace transform of a grid function $w = \{w_n\}_{n\geq 0}$ on a regular grid with time step Δt is defined for $\eta > 0$ by

$$\mathcal{L}w(s) = \widehat{w}(s) = \frac{1}{\sqrt{2\pi}}\Delta t \sum_{n\geq 0} e^{-sn\Delta t} w_n, \quad s = \eta + i\tau,\ |\tau| \leq \frac{\pi}{\Delta t}, \tag{8.1}$$

and the inversion formula is given by

$$w_n = \frac{1}{\sqrt{2\pi}} \int_{-\frac{\pi}{\Delta t}}^{\frac{\pi}{\Delta t}} e^{sn\Delta t}\widehat{w}(s)d\tau = -\frac{i}{\sqrt{2\pi}} \int_{|z|=e^{\eta\Delta t}} z^{n-1}\widehat{w}(z)dz.$$

The corresponding norms are

$$||w||_{\eta,\Delta t} = (\Delta t \sum_{n\geq 0} e^{-2\eta n\Delta t}|w_n|^2)^{\frac{1}{2}}, \qquad ||\widehat{w}||_\eta = (\int_{-\frac{\pi}{\Delta t}}^{\frac{\pi}{\Delta t}} |\widehat{w}(\eta + i\tau)|^2 d\tau)^{\frac{1}{2}} \tag{8.2}$$

and we have Parseval's equality

$$||w||_{\eta,\Delta t} = ||\widehat{w}||_\eta. \tag{8.3}$$

Suppose now $W(j,n)$ to be a solution of the difference equation

$$iD_t^+ W(j,n) + D_x^+ D_x^- W(j, n+\tfrac{1}{2}) + VW(j, n+\tfrac{1}{2}) = 0, \tag{8.4}$$

with initial condition $W(j,0) = 0$. We denote by $\widehat{W}(j,s)$ the discrete Laplace transform in time of $W(j,n)$. Equation (8.4) becomes the difference equation in one variable, s acting as a parameter

$$\widehat{W}(j-1,s) + 2(i\gamma h(z) - 1 + \Delta x^2 V)\widehat{W}(j,s) + \widehat{W}(j+1,s) = 0, \tag{8.5}$$

with $z = e^{s\Delta t}$, $h(z) = \frac{z-1}{z+1}$ and $\gamma = \Delta x^2/\Delta t$. Function h is a well-known homographic function, whose properties we summarize now:

Lemma 8.1 *1. The function h maps the circle of center O and radius 1 onto the line $\mathcal{R}e\, Z = 0$.*

2. The function h maps the exterior of the closed disk of center O and radius 1 onto the half-plane $\mathcal{R}e\, Z > 0$.

3. The function h maps any circle of center O and radius $a > 1$ onto the circle of center $(a^2+1)/(a^2-1)$ and radius $2a/(a^2-1)$.

We introduce the characteristic second order equation

$$r^2 + 2(i\gamma h(z) - 1 + \Delta x^2 V)r + 1 = 0. \tag{8.6}$$

The roots of (8.6) satisfy

$$r_+ r_- = 1, \quad r_+ + r_- = 2(1 - \Delta x^2 V - i\gamma h(z)). \tag{8.7}$$

Lemma 8.2 *For $|z| > 1$ (i.e. $\eta > 0$), equation (8.6) has two distinct roots $r_\pm$ with $|r_-| < 1 < |r_+|$. Furthermore these roots are not real.*

Proof Suppose $|z| > 1$. By (8.7), the first assertion in the lemma holds true, unless $|r_-| = |r_+| = 1$. In that case we have $r_- = \overline{r_+}$, and therefore $r_+ + r_-$ is real, which implies by (8.7) that $h(z)$ is pure imaginary. This last assertion is equivalent by Lemma 8.1 to $|z| = 1$, hence the contradiction. ■

We deduce from Lemma 8.2 that for $\eta > 0$, any solution of (8.5) is a linear combination of the powers of r_+ and r_-. Then for $\widehat{W}(\cdot, s)$, with vanishing initial data, solution to (8.5), to be square integrable in Ω_i, there must be a function $a_i(s)$ such that

$$\widehat{W}(j,s) = a_i(s) r_+^{j-\ell},\ j \leq \ell \ \text{ if } i = 1, \widehat{W}(j,s) = a_i(s) r_-^j\ j \geq 0 \text{ if } i = 2. \tag{8.8}$$

8.2 The classical Schwarz relaxation algorithm

Let U be the solution of the Crank-Nicolson scheme (7.2) in $\mathbb{N} \times \{0,\dots,N\}$. Let U_i^k be the iterates of algorithm (7.3). Then the errors $W_i^k = U_i^k - U/\Omega_i$ satisfy the same algorithm with vanishing data. Therefore, they have the form (8.8): there exists functions $a_i^k(s)$ such that

$$\widehat{W}_1^k(j,s) = a_1^k(s) r_+^{j-\ell},\ j \leq \ell\,;\ ,\widehat{W}_2^k(j,s) = a_2(s) r_-^j,\ j \geq 0. \tag{8.9}$$

The transmission conditions in (7.3) impose

$$a_1^k(s) = a_2^{k-1}(s) r_-^\ell,\ a_2^k(s) = a_1^{k-1}(s) r_-^\ell. \tag{8.10}$$

Defining the convergence factor as

$$R_D(z,\gamma,\ell) = r_-^\ell, \tag{8.11}$$

we have the formula

$$\begin{aligned} \widehat{W}_1^{2k+1}(j,\cdot) &= R_D^{2k}\widehat{W}_1^1(j,\cdot),\ \widehat{W}_1^{2k+2}(j,\cdot) = R_D^{2k+1}\widehat{W}_2^1(j,\cdot),\\ \widehat{W}_2^{2k+1}(j,\cdot) &= R_D^{2k}\widehat{W}_2^1(j,\cdot),\ \widehat{W}_2^{2k+2}(j,\cdot) = R_D^{2k+1}\widehat{W}_1^1(j,\cdot). \end{aligned} \tag{8.12}$$

Lemma 8.3 *For fixed $\eta > 0$, the convergence factor $R_D(z,\gamma,\ell)$ is bounded by*

$$|R_D(z,\gamma,\ell)| \leq \frac{1}{\left(\sqrt{\Phi^2+1}+\Phi\right)^\ell},\ \Phi = \gamma\frac{e^{\eta\Delta t}-1}{e^{\eta\Delta t}+1}. \tag{8.13}$$

When Δt and Δx tend to zero, we have the asymptotic result

$$|R_D(z,\gamma,\ell)| \lesssim 1 - \ell\eta\Delta x^2/2. \tag{8.14}$$

Proof We write $r_- = \rho e^{i\theta}$. Since $r_- r_+ = 1$, we can write by (8.7),

$$\rho e^{i\theta} + \frac{1}{\rho}e^{-i\theta} = 2(1 - \Delta x^2 V - i\gamma h(z)).$$

Taking the imaginary part we obtain

$$(\rho - \frac{1}{\rho})\sin\theta = -2\gamma \mathcal{R}e\, h(z).$$

Since $\theta \neq 0$, we can define

$$\phi = \gamma\frac{\mathcal{R}e\, h(z)}{\sin\theta}.$$

Since $\rho < 1$, ϕ is positive.

$$\rho = \sqrt{\phi^2+1} - \phi = \frac{1}{\sqrt{\phi^2+1}+\phi}.$$

Since $\eta > 0$, $\mathcal{R}e\, h(z) = \frac{|z|^2-1}{|z+1|^2}$ is positive, and therefore $\sin\theta$ is positive, and $\phi \geq \gamma\mathcal{R}e\, h(z)$. By Lemma 8.1, $\mathcal{R}e\, h(z)$ lives on the circle with center $(a^2+1)/(a^2-1)$ and radius $2a/(a^2-1)$, with $a = e^{\eta\Delta t}$. The minimum value of $\mathcal{R}e\, h(z)$ is therefore $(a-1)/(a+1)$ which yields (8.13).
Suppose now that the mesh sizes tend to zero. It is easy to see that $\Phi \approx \gamma\eta\Delta t/2$. Therefore

$$|R_D(z,\gamma,\ell)| \lesssim 1 - \ell\gamma\eta\Delta t/2,$$

and hence (8.14) by using the definition of γ.

■

We introduce the discrete norms in space and time

$$||W||_{\Omega_p,\eta,\Delta t} = (\Delta t\Delta x\sum_{j\in\Omega_i}\sum_{n\geq 0} e^{-2\eta n\Delta t}|W(j,n)|^2)^{\frac{1}{2}}. \tag{8.15}$$

Theorem 8.4 *Let V be a real constant. Let U_p^k be the iterates of algorithm (7.3). For $\eta\Delta t$ sufficiently small but non-zero, and Δx sufficiently small, we have*

$$||U_p^k - U||_{\Omega_i,\eta,\Delta t} \lesssim (1-\ell\eta\Delta x^2/2)^{k-1} \max_{p=1,2} ||U_p^1||_{\Omega_p,\eta,\Delta t}.$$

Proof By (8.12), the error W_i^k is given by $\widehat{W}_i^k(j,s) = R_D^{k-1}(z,\gamma,\ell)\widehat{W}_{i'}^1(j,s)$ for any j,s, with $i'=i$ if k is odd and $i' \neq i$ is k is even. By Lemma 8.3, we can write

$$\begin{aligned}
\|W_i^k\|^2_{\Omega_i,\eta,\Delta t} &= \int_{|z|=e^{\eta\Delta t}} |R_D(z,\gamma,\ell)|^{2(k-1)} \, \|\widehat{W}_{i'}^1(z)\|^2_{\Omega_i} \, dz \\
&\leq \sup_{|z|=e^{\eta\Delta t}} |R_D(z,\gamma,\ell)|^{2(k-1)} \int_{|z|=e^{\eta\Delta t}} \|\widehat{W}^0(z)\|^2_{\Omega_{i'}} \, dz \\
&\lesssim (1-\ell\eta\Delta x^2/2)^{2(k-1)} \, \|U_{i'}^1\|^2_{\Omega_i',\eta,\Delta t} \, .
\end{aligned}$$

■

Remark 8.5 *For $|z|=1$, when $r_\pm$ are real $|R_D(z,\gamma,\ell)|<1$. However, for $|z|=1$, when $r_\pm$ are complex conjugate $|R_D(z,\gamma,\ell)|=1$: the purely propagative modes are not damped by the overlap.*

8.3 The overlapping Robin Schwarz relaxation algorithm

We consider now algorithm (7.16,7.17,7.18) with transmission conditions (7.20). If U is the solution of the Crank-Nicolson scheme in $\mathbb{N}\times\{0,\dots,N\}$, it satisfies $B_rU(\ell,n) = \tilde{B}_rU(\ell,n) - \Delta x F(\ell, n+\frac{1}{2})$, and $B_\ell U(0,n) = \tilde{B}_\ell U(0,n) + \Delta x F(0,n+\frac{1}{2})$. Therefore the errors satisfy the algorithm with vanishing data, and we can apply the results of Section 8.1: there exist functions $a_i^k(s)$ such that

$$\widehat{W}_1^k(j,s) = a_1^k(s) r_+^{j-\ell}\ ,\ j\leq \ell\ ,\widehat{W}_2^k(j,s) = a_2(s) r_-^j\ ,\ j\geq 0. \tag{8.16}$$

The transmission conditions in (7.20) impose

$$\begin{aligned}
&a_1^k(s) = R_R(z,\gamma) a_2^{k-1}(s), a_2^k(s) = R_R(z,\gamma)a_1^{k-1}(s), with \\
&R_R(z,\gamma,p,\ell) = -R_D(z,\gamma,\ell)\frac{1-\Delta x^2 V - r_- - i\gamma h(z) + ip\Delta x}{1-\Delta x^2 V - r_- - i\gamma h(z) - ip\Delta x}
\end{aligned} \tag{8.17}$$

We already proved that $|R_D(z,\gamma,\ell)|<1$. We only need to study the other term

$$\alpha(z,\gamma,p) = \frac{1-\Delta x^2 V - r_- - i\gamma h(z) + ip\Delta x}{1-\Delta x^2 V - r_- - i\gamma h(z) - ip\Delta x}.$$

For positive p, its modulus is bounded by 1 if and only if $\mathcal{I}m\,(1-\Delta x^2V - r_- - i\gamma h(z)) \leq 0$. In the proof of Lemma 8.3, we proved that $\mathcal{R}e\, h(z) > 0$, and $\mathcal{I}m\, r_- > 0$. Therefore $|\alpha(z,\gamma,p)|<1$ for any strictly positive p.

Remark 8.6 *For $|z|=1$, when $r_\pm$ are real $|R_D(z,\gamma,\ell)|<1$ which yields $|R_R(z,\gamma,\ell)|<1$. For $|z|=1$, when $r_\pm$ are complex conjugate $|R_D(z,\gamma,\ell)|=1$ and*

$$|R_R(z,\gamma,p,\ell)| = \left|\frac{\sqrt{1-(1-\Delta x^2 V + \gamma\tan\frac{\tau\Delta t}{2})^2} - p\Delta x}{\sqrt{1-(1-\Delta x^2 V + \gamma\tan\frac{\tau\Delta t}{2})^2} + p\Delta x}\right| < 1.$$

These modes are damped, even without overlap.

Theorem 8.7 *Let V be a real constant. Let U_p^k be the iterates of algorithm (7.16,7.17,7.18). For positive p, $\eta\Delta t$ sufficiently small but non-zero, and Δx sufficiently small, we have*

$$||U_p^k - U||_{\Omega_i,\eta,\Delta t} \lesssim (1-\ell\eta\Delta x^2/2)^{k-1} \max_{p=1,2} ||U_p^1||_{\Omega_p,\eta,\Delta t}.$$

8.4 The non-overlapping Robin Schwarz relaxation algorithm

We consider now the case where $\ell = 0$. In this case, the convergence factor associated to the classical Schwarz algorithm is equal to 1. This algorithm is not convergent. For the Robin Schwarz relaxation algorithm, the convergence factor is $\alpha(z,\gamma,p)$. For $\eta > 0$ and $p > 0$, we have proved that $|\alpha(z,\gamma,p)| < 1$. This shows the convergence of the non-overlapping Robin Schwarz relaxation algorithm when V is a real constant.

However, our numerical computations are implemented with non constant potentials. Thus, we introduce a proof of convergence based on energy estimates. It is the discrete analog to the proof of Theorem 6.5. The errors are solution for $k \geq 1$ of the equations

$$iD_t^+ W_1^k(j,n) + D_x^+ D_x^- W_1^k(j,n+\tfrac{1}{2}) + V(j) W_1^k(j,n+\tfrac{1}{2}) = 0 \text{ for } -\infty < j < 0,\ 0 \leq n \leq N, \tag{8.18}$$
$$iD_t^+ W_2^k(j,n) + D_x^+ D_x^- W_2^k(j,n+\tfrac{1}{2}) + V(j) W_2^k(j,n+\tfrac{1}{2}) = 0 \text{ for } 0 < j < +\infty,\ 0 \leq n \leq N, \tag{8.19}$$

with vanishing initial values. The transmission conditions are for $k \geq 2$:

$$B_r W_1^k(0,n) = \tilde{B}_r W_2^{k-1}(0,n),\ B_\ell W_2^k(0,n) = \tilde{B}_\ell W_1^{k-1}(0,n) \text{ for } 0 \leq n \leq N, \tag{8.20}$$

where the discrete transmission operators B_j and $\tilde{B}_j$ are summarized in (7.19). The algorithm is initialized on the boundary by

$$B_r W_1^1(0,n) = \frac{\Delta x}{2}\, \tilde{G}_L(n),\ B_\ell W_2^1(n) = \frac{\Delta x}{2}\, \tilde{G}_0(n) \text{ for } 0 \leq n \leq N, \tag{8.21}$$

with $\frac{\Delta x}{2}\, \tilde{G}_L(n) = \frac{\Delta x}{2}\, G_L(n) - (B_r U(0,n) + \Delta x F(0,n+\frac{1}{2}))$ and $\frac{\Delta x}{2}\, \tilde{G}_0(n) = \frac{\Delta x}{2}\, G_0(n) - (B_\ell U(0,n) - \Delta x F(0,n+\frac{1}{2}))$. We start with the study of the discrete problem in Ω_1.

Lemma 8.8 *Let W be the solution of*

$$iD_t^+ W(j,n) + D_x^+ D_x^- W(j,n+\tfrac{1}{2}) + V(j) W(j,n+\tfrac{1}{2}) = 0 \textit{ for } -\infty < j < 0,\ 0 \leq n \leq N, \tag{8.22}$$
$$B_r W(0,n) = \frac{\Delta x}{2}\, G(n), \tag{8.23}$$

with vanishing initial data. Then we have

$$\Delta x {\sum_{j \leq 0}}' |W(j,p)|^2 + p\Delta t \sum_{0 \leq n \leq p} |W(0,n+\tfrac{1}{2})|^2 \leq \frac{1}{2p} \Delta x^2 \Delta t \sum_{0 \leq n \leq p} |G(n)|^2, \tag{8.24}$$

with the usual notation ${\sum_{j \leq 0}}' w_j = w_0/2 + \sum_{j \leq -1} w_j$.

Proof We write energy estimates, using a discrete analogous to the proof of Lemma 2.1. We multiply (8.22) by $\overline{W(j,n+\frac{1}{2})}$, take the imaginary part, and sum for $j \leq -1$. The third term vanishes due to the fact that V is real valued. The first term becomes

$$\frac{1}{2\Delta t} \sum_{j \leq -1} (|W(j,n+1)|^2 - |W(j,n)|^2). \tag{8.25}$$

As for the second term, we ignore the time for a moment, and use the fact that $D_x^+ D_x^- w_j = (D_x^- w_{j+1} - D_x^- w_j)/\Delta x$ to perform a discrete integration by parts:

$$\begin{aligned}
\sum_{j \leq -1} \overline{w_j} D_x^+ D_x^- w_j &= \frac{1}{\Delta x} \sum_{j \leq -1} \overline{w_j} (D_x^- w_{j+1} - D_x^- w_j), \\
&= \frac{1}{\Delta x} (\sum_{j \leq 0} \overline{w_{j-1}} D_x^- w_j - \sum_{j \leq -1} \overline{w_j} D_x^- w_j), \\
&= -\sum_{j \leq 0} |D_x^- w_j|^2 + \frac{1}{\Delta x} \overline{w_0} D_x^- w_0.
\end{aligned}$$

Thus we can write

$$\frac{1}{2\Delta t}\sum_{j\le -1}(|W(j,n+1)|^2-|W(j,n)|^2)+\frac{1}{\Delta x}\mathcal{I}m\,\overline{W(0,n+\tfrac12)}D_x^-W(0,n+\tfrac12)=0, \tag{8.26}$$

which we rewrite as

$$\frac{1}{2\Delta t}{\sum_{j\le 0}}'(|W(j,n+1)|^2-|W(j,n)|^2)+\frac{1}{\Delta x}\mathcal{I}m\,\left[\overline{W(0,n+\tfrac12)}(D_x^-W(0,n+\tfrac12)-i\frac{\Delta x}{2}D_t^+W(0,n))\right]=0. \tag{8.27}$$

We now multiply by $2\Delta t\Delta x$, and introduce the boundary operator B_r:

$$\Delta x{\sum_{j\le 0}}'(|W(j,n+1)|^2-|W(j,n)|^2)+2\Delta t\mathcal{I}m\,\left[\overline{W(0,n+\tfrac12)}(B_rW(0,n)+ipW(0,n+\tfrac12)\right]=0. \tag{8.28}$$

Using the boundary condition, summing in time, and using the discrete Cauchy Schwarz inequality yields (8.24). ■

Theorem 8.9 *The discrete non-overlapping Schwarz waveform relaxation algorithm (7.16,7.17,7.18) converges for $p>0$, in $l^\infty(0,N;l^2(-\infty,0))\times l^\infty(0,N;l^2(0,+\infty))$, to the solution U of (7.2), for any initial guess (G_0,G_L) and any positive p: for any n, $0\le n\le N$,*

$$\lim_{k\to+\infty}\Delta x\left[{\sum_{j\le 0}}'|(W_1^k-U)(j,n)|^2+{\sum_{j\ge 0}}'|(W_2^k-U)(j,n)|^2\right]=0. \tag{8.29}$$

Proof We first write energy estimates in each subdomain.We start with (8.27), and introduce the operators B_j. We obtain

$$\frac{1}{2\Delta t}{\sum_{j\le 0}}'(|W_1^k(j,n+1)|^2-|W_1^k(j,n)|^2)+\frac{1}{4p\Delta x}|\tilde B_\ell W_1^k(0,n)|^2=\frac{1}{4p\Delta x}|B_rW_1^k(0,n)|^2. \tag{8.30}$$

We obtain in the same way the estimates on the right

$$\frac{1}{2\Delta t}{\sum_{j\ge 0}}'(|W_2^k(j,n+1)|^2-|W_2^k(j,n)|^2)+\frac{1}{4p\Delta x}|\tilde B_rW_2^k(0,n)|^2=\frac{1}{4p\Delta x}|B_\ell W_2^k(0,n)|^2. \tag{8.31}$$

We now add (8.30) to (8.31), use the transmission conditions (8.20) for $k\ge 2$, and obtain

$$\begin{aligned}&\frac{1}{2\Delta t}{\sum_{j\le 0}}'(|W_1^k(j,n+1)|^2-|W_1^k(j,n)|^2)+\frac{1}{2\Delta t}{\sum_{j\ge 0}}'(|W_2^k(j,n+1)|^2-|W_2^k(j,n)|^2)\\&\quad+\frac{1}{4p\Delta x}(|\tilde B_rW_2^k(0,n)|^2+|\tilde B_\ell W_1^k(0,n)|^2)=\frac{1}{4p\Delta x}(|\tilde B_\ell W_1^{k-1}(0,n)|^2+|\tilde B_rW_2^{k-1}(0,n)|^2).\end{aligned} \tag{8.32}$$

We now sum up in time, for $0\le n\le p-1$:

$$\begin{aligned}&\frac{1}{2\Delta t}({\sum_{j\le 0}}'|W_1^k(j,p)|^2+{\sum_{j\ge 0}}'|W_2^k(j,p)|^2)+\frac{1}{4p\Delta x}\sum_{n=1}^{p}(|\tilde B_\ell W_1^k(0,n)|^2+|\tilde B_rW_2^k(0,n)|^2)\\&\qquad=\frac{1}{4p\Delta x}\sum_{n=1}^{p}(|\tilde B_\ell W_1^{k-1}(0,n)|^2+|\tilde B_rW_2^{k-1}(0,n)|^2).\end{aligned} \tag{8.33}$$

We finally sum up in k, for $1\le k\le K$, multiply by $2\Delta t\Delta x$, and use the boundary values for the initial guess:

$$\begin{aligned}&\sum_{k=2}^{K}\Delta x({\sum_{j\le 0}}'|W_1^k(j,p)|^2+{\sum_{j\ge 0}}'|W_2^k(j,p)|^2)+\frac{\Delta t}{2p}\sum_{n=1}^{p}(|\tilde B_\ell W_1^K(0,n)|^2+|\tilde B_rW_2^K(0,n)|^2)\\&\qquad=\frac{\Delta t}{2p}\sum_{n=1}^{p}(|\frac{\Delta x}{2}\,\tilde G_L(n)+2ipW_1^1(0,n)|^2+|\frac{\Delta x}{2}\,\tilde G_0(n)-2ipW_2^1(0,n)|^2).\end{aligned} \tag{8.34}$$

Thanks to Lemma 8.8, the right-hand side is bounded, and

$$\lim_{k\to+\infty} \Delta x\Big(\sum_{j\leq 0}{}' |W_1^k(j,p)|^2 + \sum_{j\geq 0}{}' |W_2^k(j,p)|^2\Big) = 0. \tag{8.35}$$

■

9 Numerical results

Our algorithms are implemented the Gauss-Seidel way, *i.e.* we compute u_1 with g_L, then deduce g_0 by u_1 and give it to the right domain for the computation of u_2. We compute successively $u_1^1, u_2^2, u_1^3, u_2^4, \ldots$. Thus iteration $\#k$ here corresponds to the computation of u_1^{2k-1}, u_2^{2k}.
The physical domain is $(a,b) = (-5,+5)$.

9.1 The free Schrödinger equation

In presence of an overlap, we first study the properties of the classical Schwarz algorithm, then those of the Robin algorithm, and then compare their performances. We also present the performances of the latter without overlap.

Remark 9.1 *In the case of the free Schrödinger equation, the quasi-optimal algorithm coincides with the optimal one and converges in two iterations as expected by the theory (see Theorem 4.1).*

9.1.1 The classical Schwarz algorithm

The mesh Δx and Δt are fixed, equal to $\Delta x = 0.1$ and $\Delta t = 0.01$. The overlap is equal to 8 gridpoints, *i.e* to 0.8. We compute a soliton

$$u(x,t) = \frac{e^{-i\pi/4}}{\sqrt{4t-i}}\, e^{\dfrac{ix^2 - kx - k^2 t}{4t-i}} \tag{9.1}$$

with $k = 6$, using the Crank-Nicolson scheme on (a,b) with the exacts values as Dirichlet and initial data. We study the convergence according to the finite time T, which takes values $0.5, 1, 2$. Figure 1 shows the variation of the discrete L^2 error on the boundary of Ω_2 as a function of the iteration number.

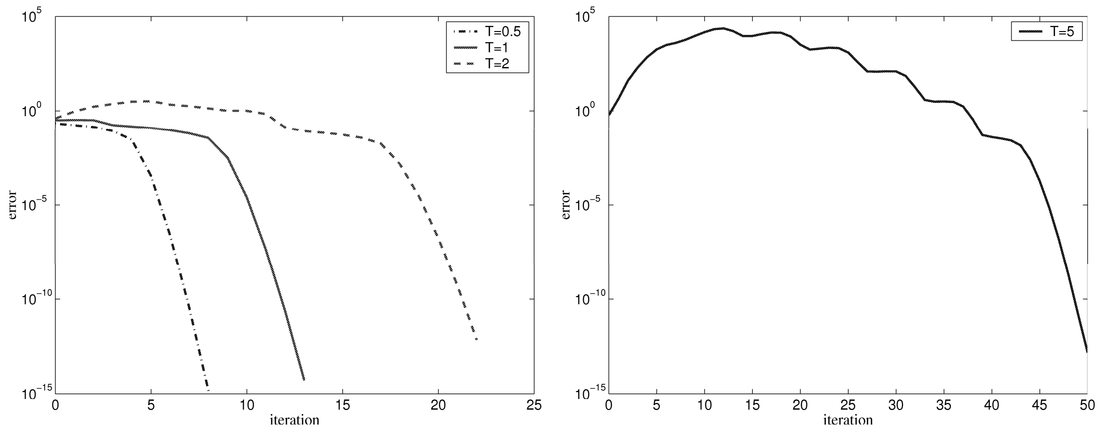

Figure 1: Convergence history of the classical Schwarz algorithm for various values of the final time.

The number of iterations needed to reach a precision equal to 10^{-12} is given in Table 1.

final time	0.5	1	2	5
number of iterations	9	14	23	51

Table 1: Number of iterations to achieve a 10^{-12} accuracy as a function of the final time for the classical Schwarz algorithm with an overlap of 8 gridpoints.

Furthermore we note that the number of iterations is not sensitive to the initial guess, as long as the compatibility condition is fulfilled. If not, then the algorithm keeps the same properties, at least for short times.

In Figure 2, we choose $T = 1$, and vary the size of the overlap from 2 to 20 gridpoints:

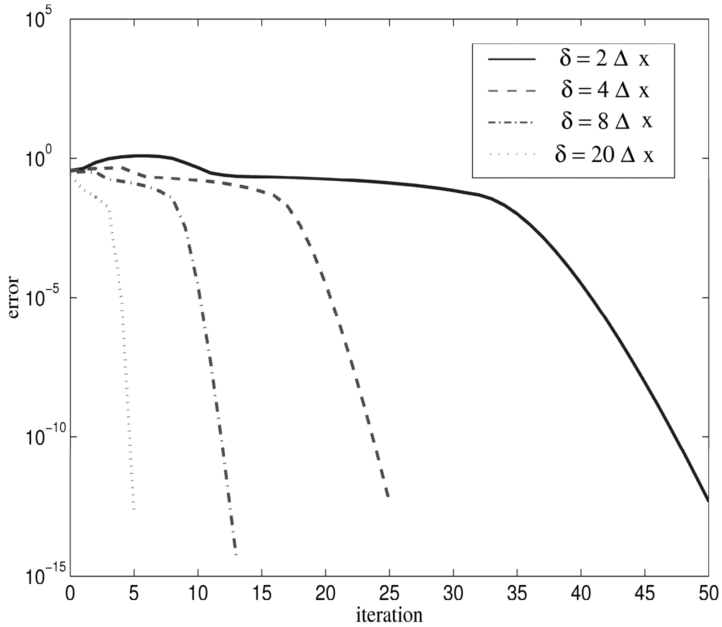

Figure 2: Convergence history of the classical Schwarz algorithm for various values of the overlap δ.

The number of iterations needed to reach a precision equal to 10^{-12} is given in Table 2.

overlap	$2\Delta x$	$4\Delta x$	$8\Delta x$	$10\Delta x$
number of iterations	51	26	14	6

Table 2: number of iterations to achieve a 10^{-12} accuracy as a function of size of the overlap for classical the Schwarz algorithm with $T = 1$.

We now choose again $T = 1$, the overlap has a fixed size 0.2 (1% of the size of the domain), and we refine in space and time, starting with $\Delta x = 0.1, \Delta t = 0.01$, and dividing both by two three times.

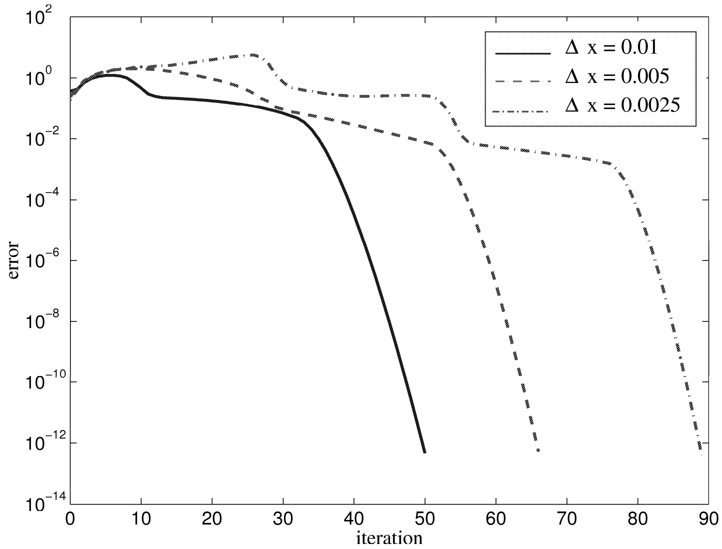

Figure 3: Convergence history of the classical Schwarz algorithm for various values of the mesh sizes. The overlap is equal to 1%.

The stagnation in the beginning of the process illustrates the theoretical result which asserts the convergence of $e^{-t}u_j^k$.

9.1.2 The optimized Robin algorithm with overlap

From now on, we consider the convergence to zero, with a random initial datum on the interface. The final time is $T = 1$, the mesh sizes are equal to $\Delta x = 0.1, \Delta t = 0.01$, and thereafter divided by two, the overlap is equal to $4\Delta x$. The optimal p given by the theory is $p_T = \left(\frac{\pi^2}{T\Delta t}\right)^{1/4}$. We draw on Figure 4 the L^2 error in Ω_1 at step 10 as a function of p. The star corresponds to p_T. This drawing shows that the performance of the Robin algorithm depends drastically on the parameter p, that the theoretical estimate is quite relevant in this case, and that it is better to overestimate p than underestimate. We show on Table 3 the values of the theoretical optimum p_T and numerical optimum p_N, together with the corresponding errors (L^2 in time and space in Ω_1).

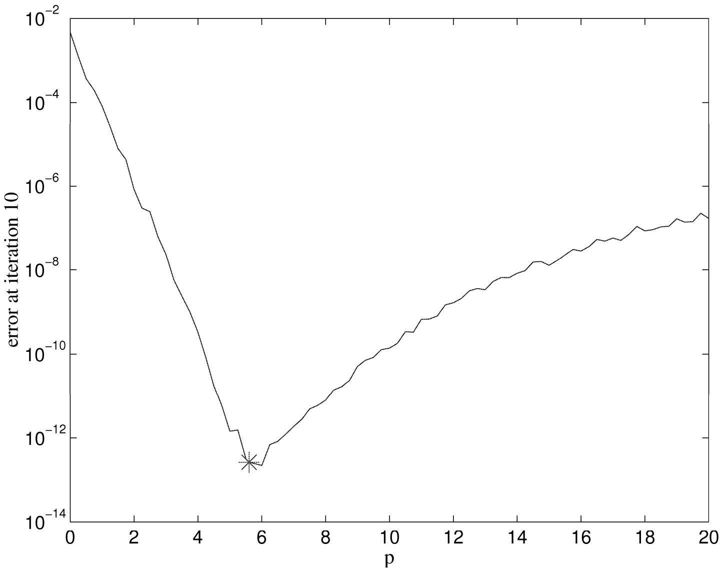

Figure 4: Variation of the quadratic error in time and space as a function of p. The overlap is equal to 1%. The star corresponds to the theoretical optimal value p_T.

Δx	0.1	0.05	0.025	0.0125
Δt	0.01	0.005	0.0025	0.00125
p_T	5.6	6.7	7.9	9.4
e_T	$0.31\,10^{-12}$	$0.31\,10^{-7}$	$0.50\,10^{-5}$	$0.48\,10^{-3}$
p_N	5.5	6.7	7.9	12.7
e_N	$0.29\,10^{-12}$	$0.31\,10^{-7}$	$0.50\,10^{-5}$	$0.0637\,10^{-3}$

Table 3: Optimal theoretical and numerical values of p after 10 iterations for various values of the mesh sizes, together with the L^2 norm of the error.

If the mesh size is not too small, then the theoretical optimal values of p is relevant. We now address the question of complex values of p. The final time is $T = 1$, $\Delta x = 0.1$ and $\Delta t = 0.01$. The overlap is equal to 4 gridpoints, *i.e* to 0.4. Figure 4 shows the equivalues of quadratic error in time and space, for a range of values of $\mathcal{R}e\,p$ and $\mathcal{I}m\,p$.

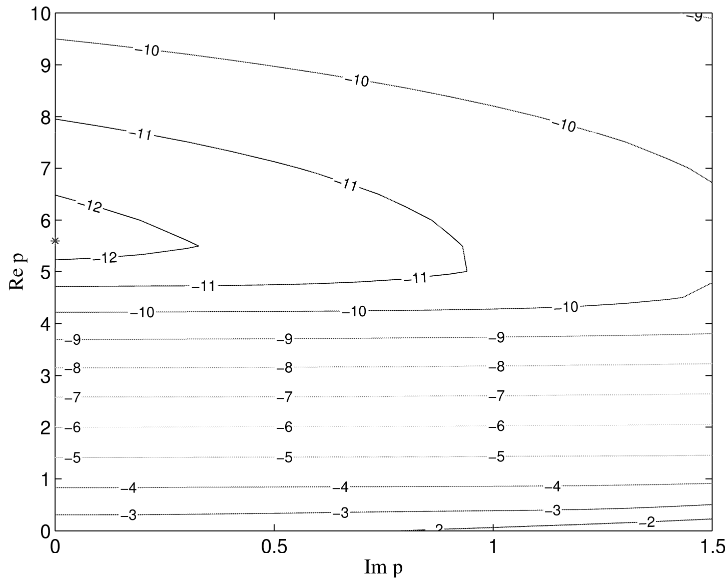

Figure 5: Variation of the quadratic error in time and space as a function of p. The overlap is equal to 4%. The star corresponds to the theoretical optimal value p_T.

It seems that adding an imaginary part to p does not improve the performance of the algorithm.

9.1.3 Comparison

We now compare the performances of the classical and optimized Robin algorithm. Since the classical algorithm converges better when the overlap is large, we consider an overlap of 8%, with the same data as in Figure 5. The error is the L^2 norm of the error on the boundary of Ω_2.

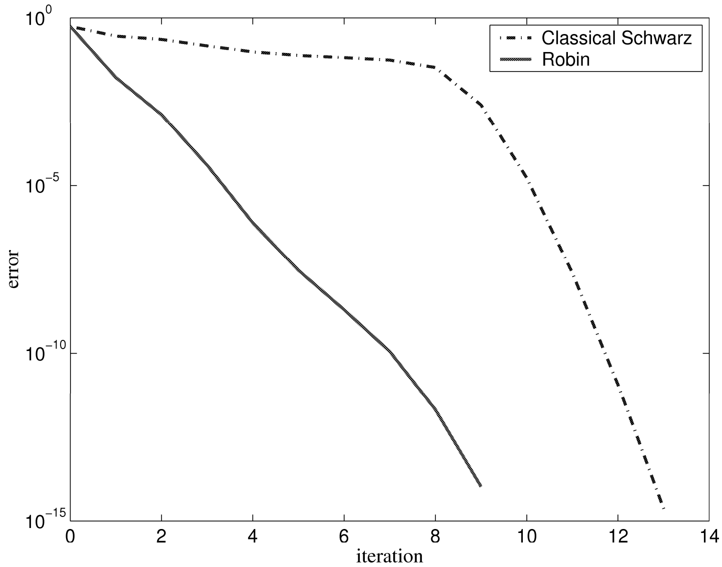

Figure 6: Convergence history: comparison of the Dirichlet and optimized Robin Schwarz algorithm. The overlap is equal to 8%.

We clearly see the improvement.

9.1.4 The optimized Robin algorithm without overlap

For the same data as before, Figure 7 shows the quadratic error in time and space in Ω_1 as a function of p for $\Delta x = 0.1, 0.05, 0.025, 0.0125$ and $\Delta t = \Delta x/10$ as before. The error is much larger than in the nonoverlapping case, and does not vary so much with p.

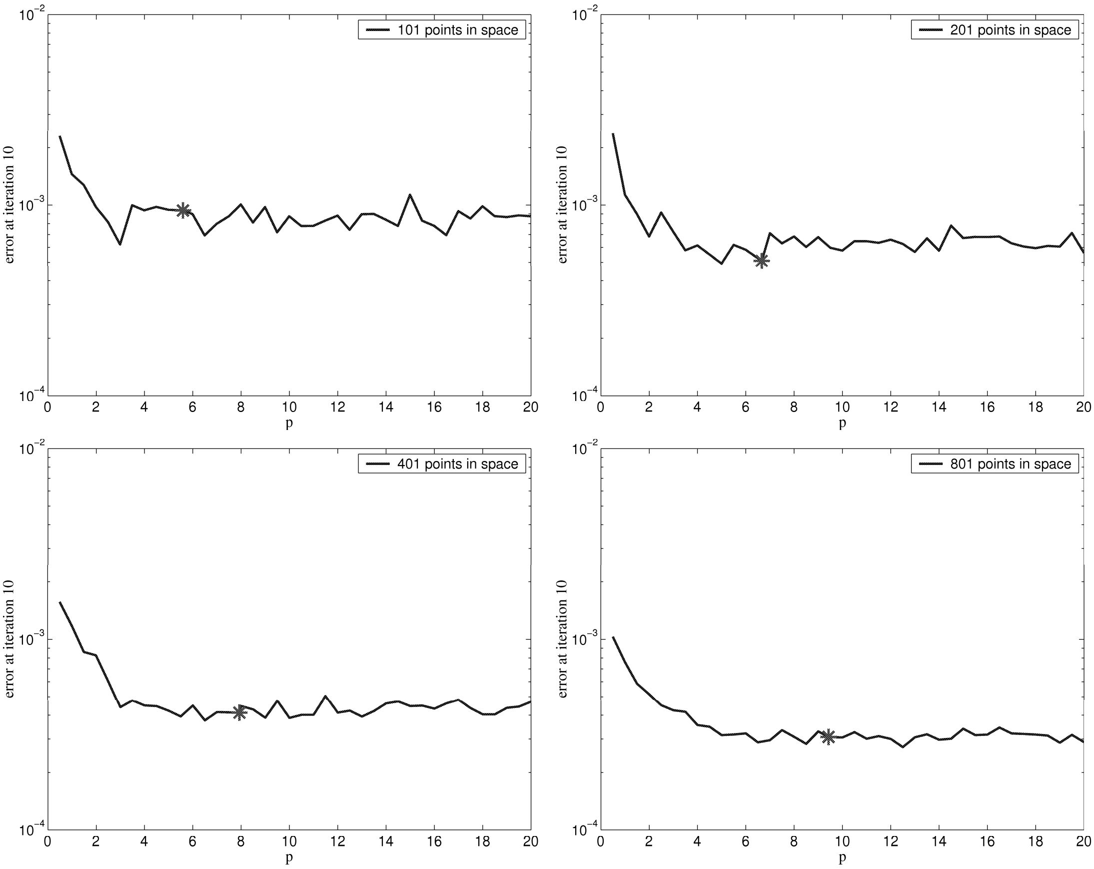

Figure 7: Error at iteration 10 as a function of p for various values of $(\Delta x, \Delta t)$. The overlap is equal to $4\Delta x$.

We draw in Figure 8 the errors of the sequences of iterates in the case $\Delta x = 0.1$, the error is the L^2 norm of the error on the boundary of Ω_2. The error decreases very fast in the beginning (reaching 10^{-8} in 5 iterations), and continues to decrease, but much slower, in the next iterations.

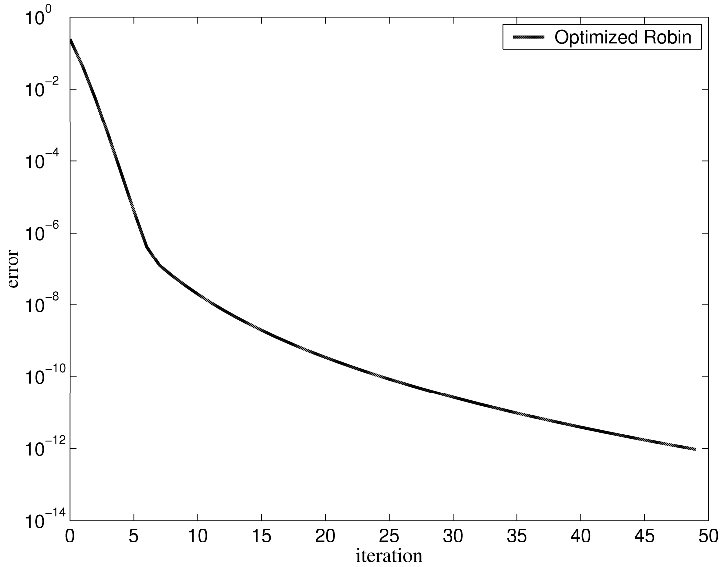

Figure 8: Convergence history for the optimized Robin Schwarz algorithm in the non overlapping case.

As in the overlapping case, adding an imaginary part to p does not improve the convergence.

9.2 The potential barrier

We consider from now on the interval $(-5, 5)$, with a final time $T = 1$, discretized with $\Delta x = 0.05$ and $\Delta t = 0.005$. The size of the overlap is $4\Delta x$. The potential is 20 times the characteristic function of the interval $(-1, 1)$. Since the potential is not a constant over the whole interval, the optimization process of Section 6.4 is irrelevant. A constant potential V equal to 20 in the formula gives a theoretical parameter p equal to 5.22. We draw in Figure 9 the error at iteration 10 as a function of p. The star corresponds to the theoretical optimal value p_T for the constant potential equal to 20. We see that the theoretical optimal value of p is the same order of magnitude as the numerical optimal value, but is not very close. However the error for the theoretical value is already small.

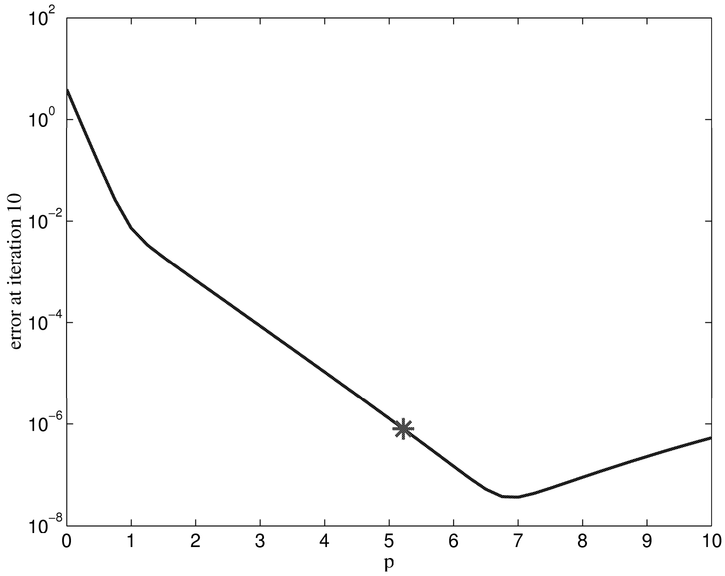

Figure 9: Error at iteration 10 as a function of p

We draw now the convergence history for Dirichlet and Robin algorithms:

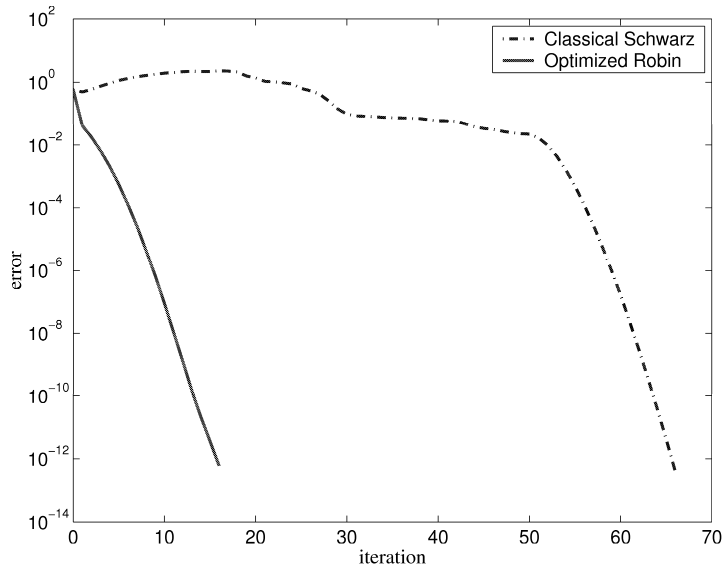

Figure 10: Convergence history: comparison of the Dirichlet and optimized Robin Schwarz algorithm for a positive potential barrier. The overlap is equal to 4%.

In this case again, the Robin condition behaves much better than the Dirichlet condition.

Note that we tried various values of the potential, like parabolic profiles and the results are the same Robin algorithm behaves much better than Schwarz, and the optimal Robin is obtained for a value of the parameter of the same order of magnitude as the theoretical one.

9.3 The quasi-optimal algorithm

The quasi optimal algorithm is by far the most efficient. In all cases, even when the potential is not constant, the precision 10^{-12} is reached in at most five iterations with or without overlap. As an example, we show in Figure 11 the convergence history with an overlap of 8 gridpoints, for a linear potential equal to $10x$.

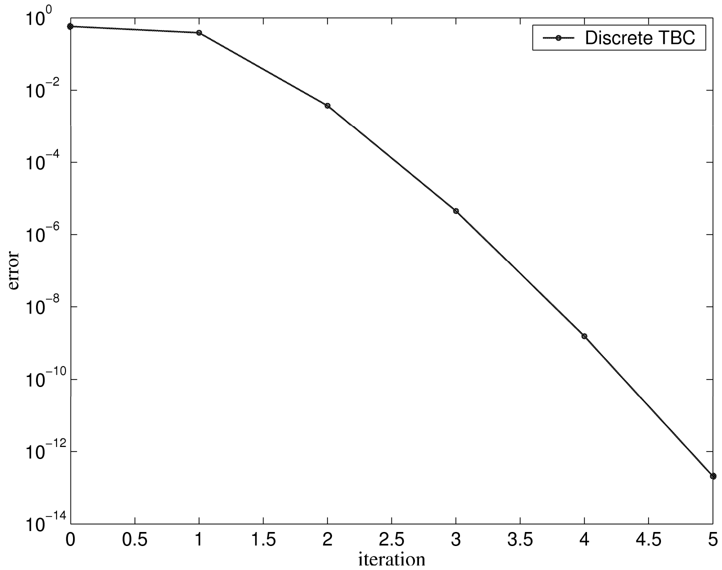

Figure 11: Convergence history for the quasi-optimal Schwarz algorithm in presence of a linear potential

In Figure 12, we show the first few iterations, at the end of the time interval, of the quasi optimal algorithm with a parabolic potential.

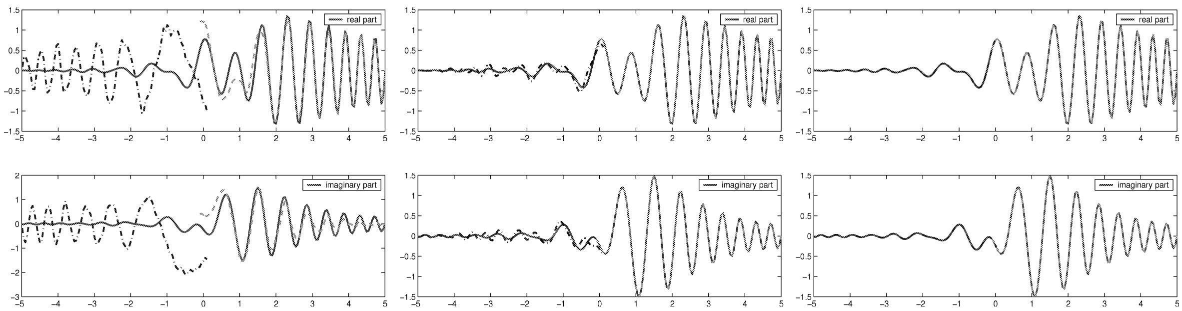

Figure 12: From left to right, the iterates $u_1^k(x,T)$ and $u_2^{k+1}(x,T)$ (dashed) at the end of the time interval $t = T$ for $k = 1, 3, 5$, together with the exact solution (solid).

10 Conclusion

We have presented here a general approach to design optimized and quasi-optimal domain decomposition algorithms for the linear Schrödinger equation with a potential in one dimension. It allows the use of any discretization, any time and space steps in the subdomains. These algorithms greatly improve the performances of the classical Schwarz relaxation algorithm. We intend to extend our analysis to the two-dimensional case in a close future.

References

[1] A. Arnold and M. Ehrhardt. Discrete transparent boundary conditions for the Schrödinger equation. *Rivista di Mathematica della Universita di Parma*, 6(4):57–108, 2001.

[2] D.Bennequin, M. Gander, and L. Halpern. Optimized Schwarz waveform relaxation for convection reaction diffusion problems. Technical Report 2004-24, LAGA, Université Paris 13, 2004. http://www-math.math.univ-paris13.fr/prepub/pp2004/pp2004-24.html.

[3] B. Després. *Méthodes de décomposition de domaines pour les problèmes de propagation d'ondes en régime harmonique*. PhD thesis, Université Paris IX Dauphine, 1991.

[4] Martin J. Gander and Hongkai Zhao. Overlapping Schwarz waveform relaxation for parabolic problems in higher dimension. In A. Handlovičová, Magda Komorníkova, and Karol Mikula, editors, *Proceedings of Algoritmy 14*, pages 42–51. Slovak Technical University, September 1997.

[5] M.J. Gander, L. Halpern, and F. Nataf. Optimal Schwarz waveform relaxation for the one dimensional wave equation. *SIAM Journal on Numerical Analysis*, 41:1643–1681, 2003.

[6] Jacques-Louis Lions and Enrico Magenes. *Problèmes aux limites non homogènes et applications*, volume 17-18 of *Travaux et recherches mathématiques*. Dunod, 1968.

[7] Pierre-Louis Lions. On the Schwarz alternating method. III: a variant for nonoverlapping subdomains. In Tony F. Chan, Roland Glowinski, Jacques Périaux, and Olof Widlund, editors, *Third International Symposium on Domain Decomposition Methods for Partial Differential Equations , held in Houston, Texas, March 20-22, 1989*, Philadelphia, PA, 1990. SIAM.

[8] Frédéric Nataf, Francois Rogier, and Eric de Sturler. Optimal interface conditions for domain decomposition methods. Technical Report 301, CMAP (Ecole Polytechnique), 1994.

[9] Walter Rudin. *Real and Complex Analysis*. Mc Graw-Hill, 1966.

[10] John C. Strikwerda. *Finite Difference Schemes and Partial Differential Equations*. Chapman and Hall, 1989.

[11] J. Szeftel. Design of absorbing boundary conditions for the linear Schrödinger equation in $\mathbb{R}^d$. *SIAM Journal on Numerical Analysis*, 42:1527–1551, 2004.